Supporting Information for

Synthesis and Activity of Ruthenium Olefin Metathesis Catalysts Coordinated with Thiazol-2-ylidene Ligands

by

Georgios C. Vougioukalakis, and Robert H. Grubbs*

Arnold and Mabel Beckman Laboratory of Chemical Synthesis, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125

Crystallographic Analysis

[$RuCl_2$ (3-phenyl-4,5-dimethylthiazol-2-ylidene) (=CH-*o*-*i*PrO-Ph)] (6)

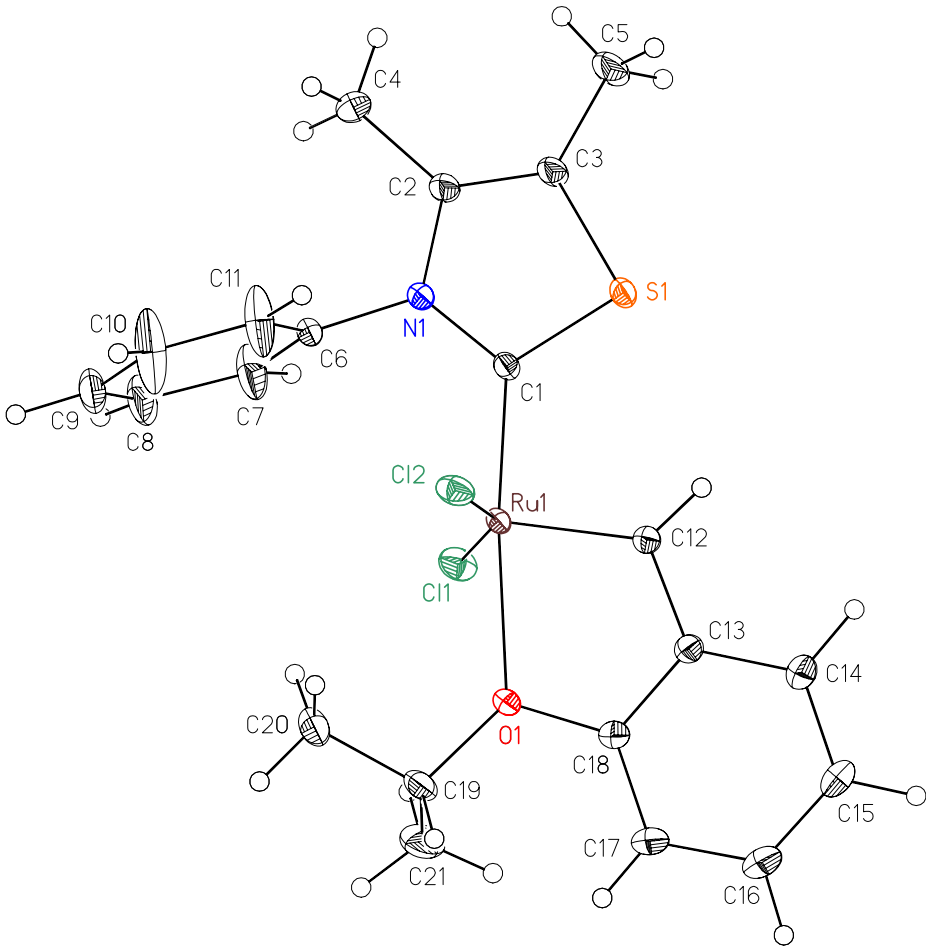


Table 1. Crystal data and structure refinement for CCDC 642800.

Empirical formula	$C_{21}H_{23}NOSClRu$
Formula weight	509.43
Crystallization Solvent	Hexanes/deuteratedbenzene
Crystal Habit	Plate
Crystal size	0.44 x 0.36 x 0.11 mm^3
Crystal color	Brown

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 27295 reflections used in lattice determination	2.54 to 46.26°
Unit cell dimensions	a = 8.6637(3) Å b = 23.1580(7) Å β= 99.6310(10)° c = 10.7183(3) Å
Volume	2120.15(11) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.596 Mg/m^3
F(000)	1032
Data collection program	Bruker SMART v5.630
θ range for data collection	1.76 to 46.38°
Completeness to θ = 46.38°	93.5 %
Index ranges	$-17 \le h \le 15$, $-36 \le k \le 47$, $-21 \le l \le 21$
Data collection scan type	ω scans at 7 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	66368
Independent reflections	17553 [R_{int}= 0.0916]
Absorption coefficient	1.101 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8885 and 0.6430

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	17553 / 0 / 336
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.278
Final R indices [$I>2\sigma(I)$, 12405 reflections]	R1 = 0.0432, *w*R2 = 0.0799
R indices (all data)	R1 = 0.0685, *w*R2 = 0.0836
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	3.779 and -1.566 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

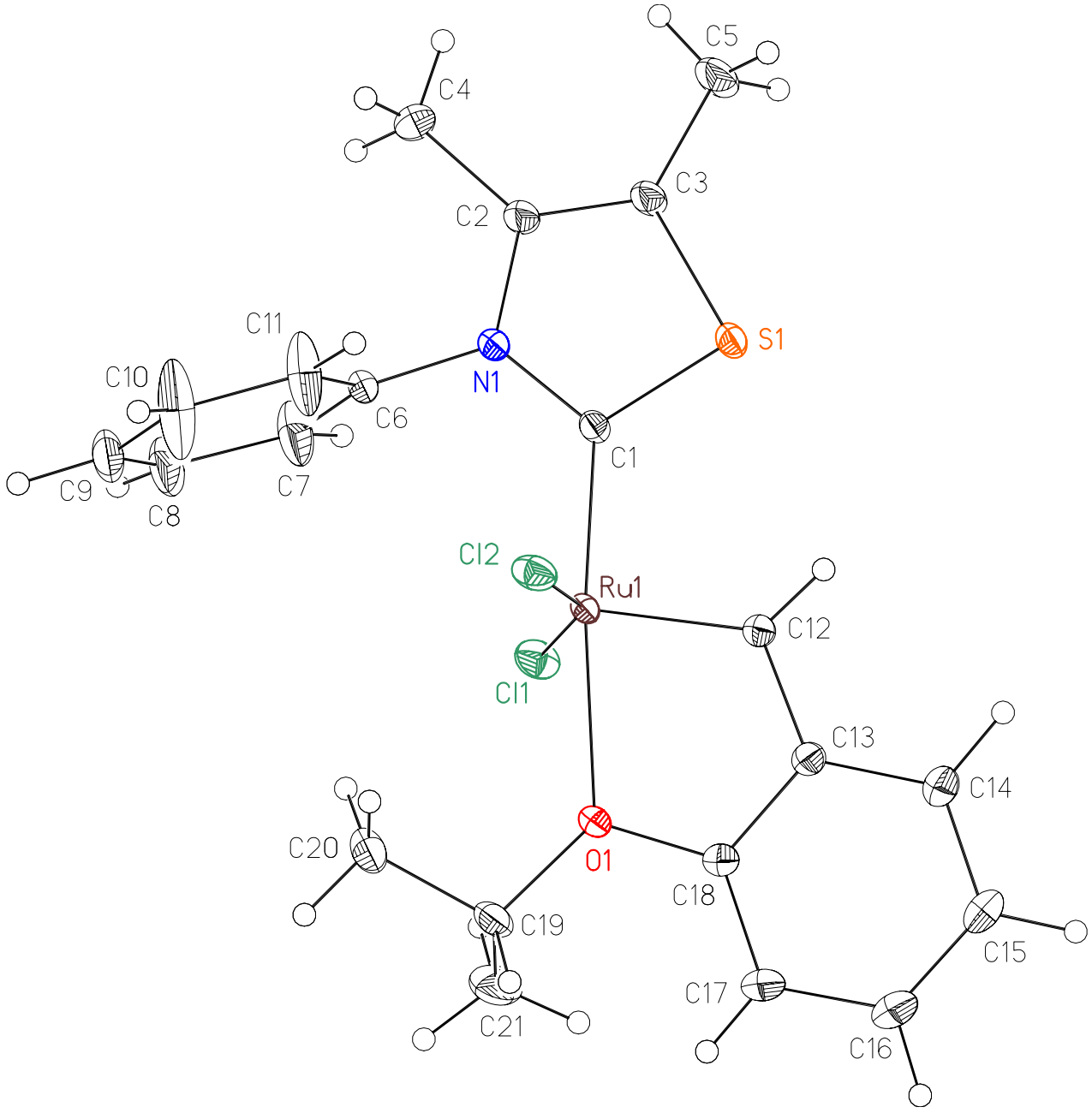

C5
C4
C3
C2
C11
S1
C10
N1
C6
C1
C9
C7
C8
Cl2
Ru1
C12
Cl1
C13
C14
C20
O1
C18
C19
C15
C17
C21
C16

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CCDC 642800. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	4263(1)	840(1)	6801(1)	11(1)
Cl(1)	2371(1)	1562(1)	6855(1)	19(1)
Cl(2)	6586(1)	348(1)	7564(1)	19(1)
S(1)	4759(1)	1170(1)	3916(1)	15(1)
O(1)	3039(1)	307(1)	8113(1)	16(1)
N(1)	6212(1)	1708(1)	5761(1)	14(1)
C(1)	5177(1)	1263(1)	5536(1)	12(1)
C(2)	6677(2)	1971(1)	4698(1)	17(1)
C(3)	5985(2)	1726(1)	3601(1)	17(1)
C(4)	7814(2)	2463(1)	4884(2)	28(1)
C(5)	6186(2)	1872(1)	2280(1)	26(1)
C(6)	6755(2)	1922(1)	7021(1)	14(1)
C(7)	5919(2)	2350(1)	7508(2)	31(1)
C(8)	6484(2)	2587(1)	8690(2)	32(1)
C(9)	7847(2)	2387(1)	9385(2)	27(1)
C(10)	8672(3)	1960(1)	8890(2)	52(1)
C(11)	8142(2)	1723(1)	7706(2)	38(1)
C(12)	3236(2)	318(1)	5673(1)	13(1)
C(13)	2239(1)	-108(1)	6131(1)	14(1)
C(14)	1353(2)	-510(1)	5327(1)	17(1)
C(15)	381(2)	-900(1)	5807(2)	24(1)
C(16)	301(2)	-895(1)	7095(2)	29(1)
C(17)	1174(2)	-503(1)	7915(2)	26(1)
C(18)	2128(2)	-108(1)	7425(1)	16(1)
C(19)	2825(2)	424(1)	9421(1)	19(1)
C(20)	4185(2)	797(1)	10000(2)	25(1)
C(21)	1258(2)	719(1)	9431(2)	29(1)

Table 3. Selected bond lengths [Å] and angles [°] for CCDC 642800.

Ru(1)-C(12)	1.8322(13)	C(12)-Ru(1)-C(1)	94.69(5)
Ru(1)-C(1)	1.9442(11)	C(12)-Ru(1)-O(1)	79.81(4)
Ru(1)-O(1)	2.2647(9)	C(1)-Ru(1)-O(1)	174.33(4)
Ru(1)-Cl(2)	2.3391(4)	C(12)-Ru(1)-Cl(2)	101.74(4)
Ru(1)-Cl(1)	2.3476(3)	C(1)-Ru(1)-Cl(2)	93.58(4)
		O(1)-Ru(1)-Cl(2)	88.92(3)
		C(12)-Ru(1)-Cl(1)	102.80(4)
		C(1)-Ru(1)-Cl(1)	91.55(4)
		O(1)-Ru(1)-Cl(1)	88.36(3)
		Cl(2)-Ru(1)-Cl(1)	154.410(14)

Table 4. Bond lengths [Å] and angles [°] for CCDC 642800.

Ru(1)-C(12)	1.8322(13)	C(21)-H(21B)	0.95(2)
Ru(1)-C(1)	1.9442(11)	C(21)-H(21C)	0.97(2)
Ru(1)-O(1)	2.2647(9)		
Ru(1)-Cl(2)	2.3391(4)	C(12)-Ru(1)-C(1)	94.69(5)
Ru(1)-Cl(1)	2.3476(3)	C(12)-Ru(1)-O(1)	79.81(4)
S(1)-C(1)	1.7271(12)	C(1)-Ru(1)-O(1)	174.33(4)
S(1)-C(3)	1.7377(14)	C(12)-Ru(1)-Cl(2)	101.74(4)
O(1)-C(18)	1.3754(17)	C(1)-Ru(1)-Cl(2)	93.58(4)
O(1)-C(19)	1.4698(15)	O(1)-Ru(1)-Cl(2)	88.92(3)
N(1)-C(1)	1.3599(16)	C(12)-Ru(1)-Cl(1)	102.80(4)
N(1)-C(2)	1.4091(16)	C(1)-Ru(1)-Cl(1)	91.55(4)
N(1)-C(6)	1.4425(16)	O(1)-Ru(1)-Cl(1)	88.36(3)
C(2)-C(3)	1.3524(19)	Cl(2)-Ru(1)-Cl(1)	154.410(14)
C(2)-C(4)	1.497(2)	C(1)-S(1)-C(3)	94.07(6)
C(3)-C(5)	1.4938(18)	C(18)-O(1)-C(19)	119.12(10)
C(4)-H(4A)	0.96(3)	C(18)-O(1)-Ru(1)	109.55(7)
C(4)-H(4B)	0.95(3)	C(19)-O(1)-Ru(1)	129.69(8)
C(4)-H(4C)	0.94(3)	C(1)-N(1)-C(2)	117.00(11)
C(5)-H(5A)	0.94(3)	C(1)-N(1)-C(6)	121.89(10)
C(5)-H(5B)	0.89(2)	C(2)-N(1)-C(6)	121.03(11)
C(5)-H(5C)	0.98(3)	N(1)-C(1)-S(1)	107.06(8)
C(6)-C(11)	1.378(2)	N(1)-C(1)-Ru(1)	126.23(9)
C(6)-C(7)	1.379(2)	S(1)-C(1)-Ru(1)	126.64(7)
C(7)-C(8)	1.393(2)	C(3)-C(2)-N(1)	112.09(12)
C(7)-H(7)	1.06(3)	C(3)-C(2)-C(4)	128.39(12)
C(8)-C(9)	1.367(3)	N(1)-C(2)-C(4)	119.52(12)
C(8)-H(8)	0.92(3)	C(2)-C(3)-C(5)	128.61(13)
C(9)-C(10)	1.377(3)	C(2)-C(3)-S(1)	109.77(9)
C(9)-H(9)	0.98(3)	C(5)-C(3)-S(1)	121.61(11)
C(10)-C(11)	1.388(3)	C(2)-C(4)-H(4A)	113.0(14)
C(10)-H(10)	0.94(3)	C(2)-C(4)-H(4B)	120.3(19)
C(11)-H(11)	0.92(3)	H(4A)-C(4)-H(4B)	103(2)
C(12)-C(13)	1.4496(17)	C(2)-C(4)-H(4C)	110.1(15)
C(12)-H(12)	0.93(2)	H(4A)-C(4)-H(4C)	103(2)
C(13)-C(18)	1.4064(17)	H(4B)-C(4)-H(4C)	106(2)
C(13)-C(14)	1.4078(19)	C(3)-C(5)-H(5A)	110.9(18)
C(14)-C(15)	1.390(2)	C(3)-C(5)-H(5B)	113.2(16)
C(14)-H(14)	1.01(2)	H(5A)-C(5)-H(5B)	109(2)
C(15)-C(16)	1.394(2)	C(3)-C(5)-H(5C)	106.3(18)
C(15)-H(15)	0.98(2)	H(5A)-C(5)-H(5C)	115(2)
C(16)-C(17)	1.395(2)	H(5B)-C(5)-H(5C)	102(2)
C(16)-H(16)	0.94(3)	C(11)-C(6)-C(7)	120.33(14)
C(17)-C(18)	1.3923(18)	C(11)-C(6)-N(1)	120.12(13)
C(17)-H(17)	0.92(2)	C(7)-C(6)-N(1)	119.46(13)
C(19)-C(20)	1.509(2)	C(6)-C(7)-C(8)	119.99(16)
C(19)-C(21)	1.522(2)	C(6)-C(7)-H(7)	118.2(19)
C(19)-H(19)	0.98(2)	C(8)-C(7)-H(7)	121.6(19)
C(20)-H(20A)	0.99(2)	C(9)-C(8)-C(7)	120.15(16)
C(20)-H(20B)	0.94(2)	C(9)-C(8)-H(8)	118.8(16)
C(20)-H(20C)	1.02(3)	C(7)-C(8)-H(8)	120.6(17)
C(21)-H(21A)	0.92(3)	C(8)-C(9)-C(10)	119.35(16)

C(8)-C(9)-H(9)	116.6(13)
C(10)-C(9)-H(9)	124.0(14)
C(9)-C(10)-C(11)	121.43(19)
C(9)-C(10)-H(10)	118(2)
C(11)-C(10)-H(10)	120(2)
C(6)-C(11)-C(10)	118.73(17)
C(6)-C(11)-H(11)	117.1(17)
C(10)-C(11)-H(11)	124.2(17)
C(13)-C(12)-Ru(1)	118.47(9)
C(13)-C(12)-H(12)	112.4(14)
Ru(1)-C(12)-H(12)	128.9(13)
C(18)-C(13)-C(14)	118.93(11)
C(18)-C(13)-C(12)	118.50(12)
C(14)-C(13)-C(12)	122.56(11)
C(15)-C(14)-C(13)	120.34(13)
C(15)-C(14)-H(14)	121.8(13)
C(13)-C(14)-H(14)	117.9(13)
C(14)-C(15)-C(16)	119.69(14)
C(14)-C(15)-H(15)	120.8(13)
C(16)-C(15)-H(15)	119.5(13)
C(15)-C(16)-C(17)	121.12(14)
C(15)-C(16)-H(16)	121.9(18)
C(17)-C(16)-H(16)	116.9(18)
C(18)-C(17)-C(16)	118.97(14)
C(18)-C(17)-H(17)	121.8(13)
C(16)-C(17)-H(17)	119.2(13)
O(1)-C(18)-C(17)	125.44(12)
O(1)-C(18)-C(13)	113.61(11)
C(17)-C(18)-C(13)	120.95(13)
O(1)-C(19)-C(20)	106.46(10)
O(1)-C(19)-C(21)	110.17(13)
C(20)-C(19)-C(21)	112.05(14)
O(1)-C(19)-H(19)	107.6(12)
C(20)-C(19)-H(19)	109.9(12)
C(21)-C(19)-H(19)	110.4(11)
C(19)-C(20)-H(20A)	112.2(13)
C(19)-C(20)-H(20B)	106.1(13)
H(20A)-C(20)-H(20B)	111.1(18)
C(19)-C(20)-H(20C)	112.1(12)
H(20A)-C(20)-H(20C)	107.9(18)
H(20B)-C(20)-H(20C)	107.3(19)
C(19)-C(21)-H(21A)	110.2(15)
C(19)-C(21)-H(21B)	111.7(13)
H(21A)-C(21)-H(21B)	99(2)
C(19)-C(21)-H(21C)	113.5(14)
H(21A)-C(21)-H(21C)	105(2)
H(21B)-C(21)-H(21C)	115.7(18)

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for CCDC 642800. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	143(1)	118(1)	83(1)	-10(1)	29(1)	-12(1)
Cl(1)	265(2)	139(1)	200(1)	-2(1)	102(1)	37(1)
Cl(2)	154(1)	276(2)	135(1)	53(1)	24(1)	14(1)
S(1)	216(1)	140(1)	94(1)	-7(1)	24(1)	-30(1)
O(1)	202(4)	166(4)	115(4)	-28(3)	65(3)	-51(3)
N(1)	177(4)	129(4)	105(4)	-8(3)	38(3)	-30(4)
C(1)	154(5)	108(4)	99(4)	-4(3)	28(3)	3(4)
C(2)	256(6)	148(5)	128(5)	4(4)	58(4)	-50(5)
C(3)	270(6)	126(5)	119(5)	11(4)	57(4)	-27(5)
C(4)	419(9)	235(7)	214(7)	-14(5)	109(6)	-181(7)
C(5)	442(9)	209(7)	128(5)	28(4)	88(6)	-55(7)
C(6)	179(5)	140(5)	102(4)	-16(3)	30(4)	-33(4)
C(7)	217(7)	427(11)	275(8)	-212(7)	-16(5)	73(7)
C(8)	267(7)	421(10)	279(8)	-228(7)	62(6)	-7(7)
C(9)	404(9)	232(7)	157(6)	-64(5)	-5(6)	-74(7)
C(10)	640(15)	366(11)	417(12)	-227(9)	-311(11)	227(11)
C(11)	405(10)	321(9)	337(10)	-204(8)	-170(8)	172(8)
C(12)	152(5)	124(5)	123(4)	-5(3)	34(4)	-14(4)
C(13)	139(5)	130(5)	145(5)	-6(4)	34(4)	-12(4)
C(14)	174(5)	142(5)	189(6)	-8(4)	15(4)	-17(4)
C(15)	233(6)	197(7)	278(7)	-26(5)	38(5)	-97(5)
C(16)	320(8)	271(8)	310(8)	-33(6)	130(6)	-157(7)
C(17)	319(7)	269(8)	225(7)	-21(5)	138(6)	-132(6)
C(18)	160(5)	169(5)	154(5)	-10(4)	55(4)	-28(4)
C(19)	282(6)	190(6)	121(5)	-5(4)	81(4)	-16(5)
C(20)	359(8)	246(7)	144(5)	-44(5)	47(5)	-61(6)
C(21)	317(8)	298(8)	295(8)	-45(6)	195(7)	-1(7)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CCDC 642800.

	x	y	z	U_{iso}
H(4A)	7970(30)	2639(11)	4100(20)	33(6)
H(4B)	8860(30)	2403(13)	5310(30)	62(9)
H(4C)	7410(30)	2768(11)	5310(30)	37(7)
H(5A)	6690(30)	2229(12)	2250(30)	46(7)
H(5B)	5290(30)	1876(11)	1740(20)	32(6)
H(5C)	6720(30)	1542(14)	1970(30)	58(9)
H(7)	4900(30)	2514(15)	6930(30)	71(10)
H(8)	6020(30)	2908(13)	8970(30)	50(8)
H(9)	8170(20)	2561(11)	10230(20)	33(6)
H(10)	9540(30)	1795(15)	9410(30)	70(10)
H(11)	8650(30)	1433(13)	7350(30)	56(8)
H(12)	3310(20)	264(10)	4830(20)	26(5)
H(14)	1430(20)	-500(10)	4390(20)	27(6)
H(15)	-260(20)	-1177(10)	5250(20)	23(5)
H(16)	-340(30)	-1154(12)	7450(30)	50(8)
H(17)	1110(20)	-512(10)	8760(20)	22(5)
H(19)	2860(20)	51(9)	9870(20)	21(5)
H(20A)	5210(20)	620(10)	9930(20)	22(5)
H(20B)	4080(20)	848(10)	10860(20)	25(6)
H(20C)	4140(20)	1198(11)	9590(20)	33(6)
H(21A)	1230(30)	1067(12)	9020(30)	36(7)
H(21B)	1160(20)	850(9)	10250(20)	22(5)
H(21C)	370(30)	503(11)	8980(20)	35(6)

[$RuCl_2$ (3-(2-methylphenyl)-4,5-dimethylthiazol-2-ylidene) (=CH-*o*-*i*PrO-Ph)] (7)

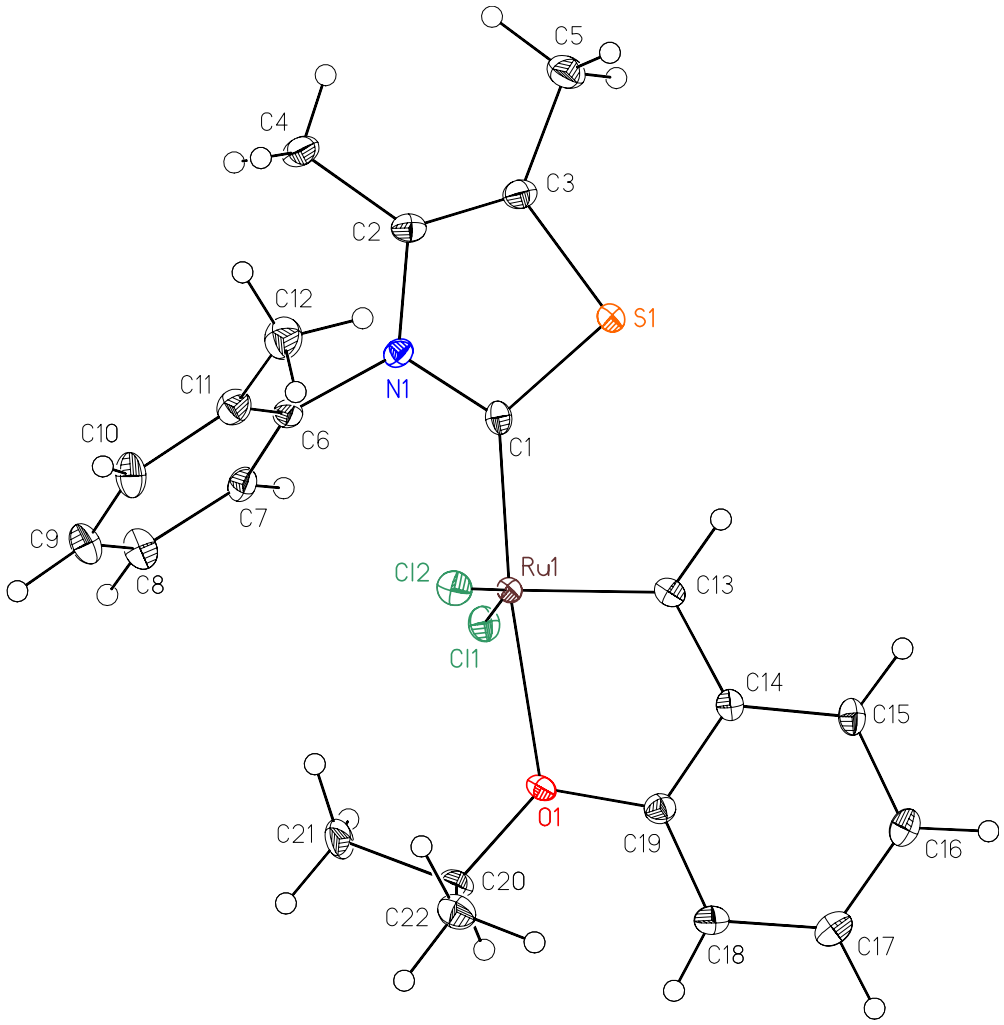


Table 1. Crystal data and structure refinement for CCDC 642801.

Empirical formula	$C_{22}H_{25}NOSCl_2Ru$
Formula weight	523.46
Crystallization Solvent	Hexanes/deuteratedbenzene
Crystal Habit	Triangular
Crystal size	0.27 x 0.23 x 0.18 mm^3
Crystal color	Brown

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 17769 reflections used in lattice determination	2.32 to 39.90°
Unit cell dimensions	a = 9.7492(3) Å b = 11.2812(4) Å c = 20.1232(6) Å
Volume	2213.20(12) $Å^3$
Z	4
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Density (calculated)	1.571 Mg/m^3
F(000)	1064
Data collection program	Bruker SMART v5.630
θ range for data collection	2.02 to 40.55°
Completeness to θ = 40.55°	94.8 %
Index ranges	$-17 \le h \le 15$, $-20 \le k \le 15$, $-36 \le l \le 36$
Data collection scan type	ω scans at 5 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	48121
Independent reflections	12769 [R_{int}= 0.0912]
Absorption coefficient	1.057 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8325 and 0.7634

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	12769 / 0 / 353
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.079
Final R indices [$I>2\sigma(I)$, 9250 reflections]	R1 = 0.0426, *w*R2 = 0.0669
R indices (all data)	R1 = 0.0668, *w*R2 = 0.0707
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Absolute structure determination	Anomalous differences
Absolute structure parameter	-0.03(2)
Largest diff. peak and hole	1.424 and -1.930 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

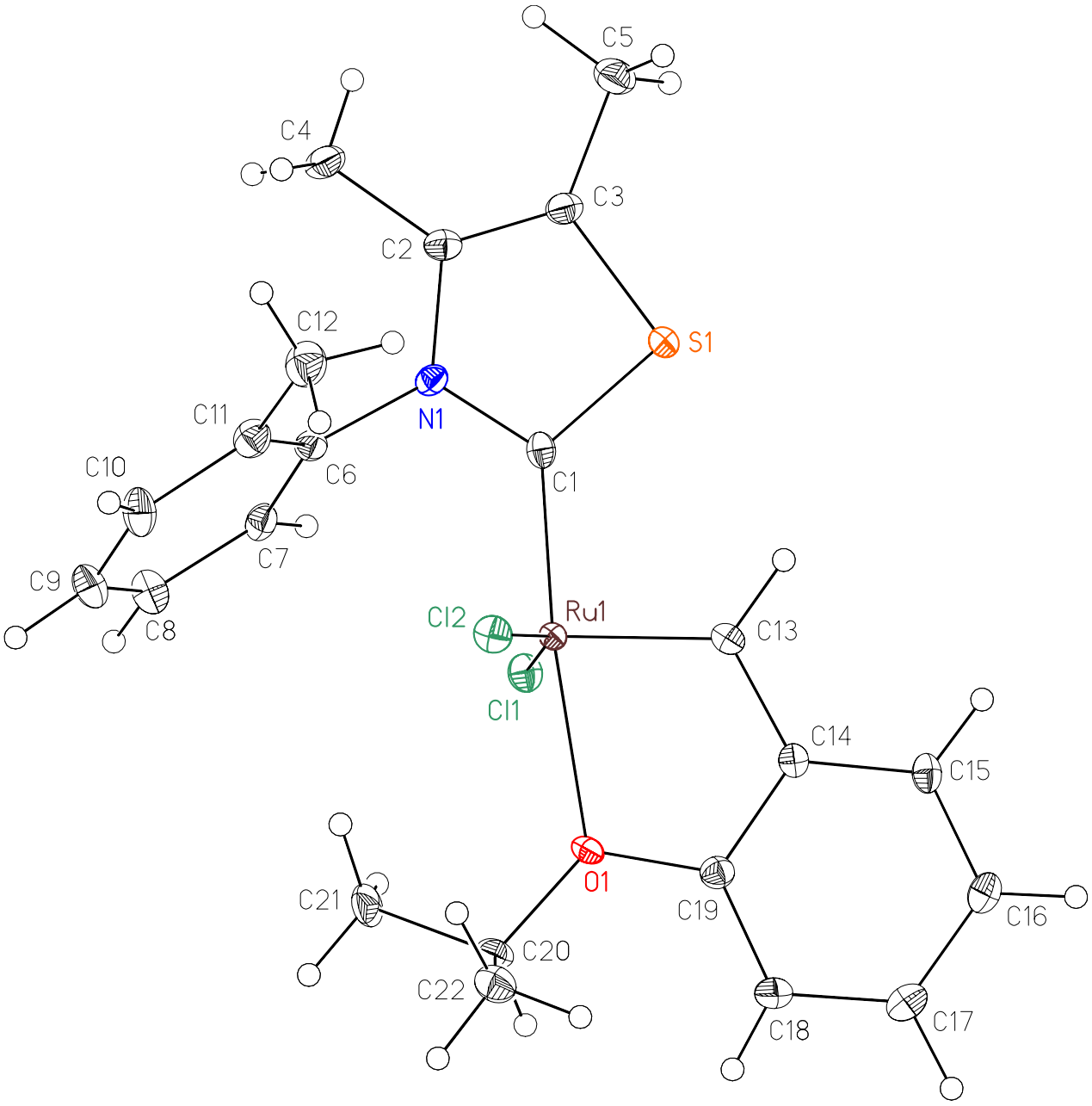

C5
C4
C3
C2
C12
S1
N1
C11
C6
C1
C10
C7
C9
C8
Cl2
Ru1
C13
Cl1
C14
C15
O1
C21
C19
C16
C20
C22
C18
C17

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CCDC 642801. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	457(1)	-52(1)	8987(1)	9(1)
Cl(1)	-394(1)	204(1)	10072(1)	14(1)
Cl(2)	1055(1)	536(1)	7917(1)	14(1)
O(1)	2450(2)	793(1)	9326(1)	12(1)
N(1)	-2248(2)	-437(2)	8362(1)	11(1)
S(1)	-1426(1)	-2436(1)	8709(1)	14(1)
C(1)	-1140(2)	-925(2)	8672(1)	11(1)
C(2)	-3298(2)	-1224(2)	8158(1)	13(1)
C(3)	-3001(2)	-2354(2)	8307(1)	14(1)
C(4)	-4599(3)	-743(2)	7863(1)	17(1)
C(5)	-3853(3)	-3432(2)	8192(2)	19(1)
C(6)	-2307(2)	836(2)	8267(1)	13(1)
C(7)	-2432(2)	1544(2)	8844(1)	14(1)
C(8)	-2423(3)	2764(2)	8786(1)	19(1)
C(9)	-2279(3)	3273(2)	8162(1)	20(1)
C(10)	-2156(3)	2575(2)	7608(1)	19(1)
C(11)	-2167(2)	1326(2)	7638(1)	16(1)
C(12)	-1960(3)	604(2)	7026(1)	21(1)
C(13)	1522(2)	-1370(2)	9096(1)	11(1)
C(14)	2916(2)	-1240(2)	9333(1)	11(1)
C(15)	3806(3)	-2187(2)	9445(1)	13(1)
C(16)	5140(2)	-2005(2)	9666(1)	16(1)
C(17)	5590(3)	-847(2)	9783(1)	18(1)
C(18)	4732(2)	120(2)	9675(1)	16(1)
C(19)	3397(2)	-76(2)	9451(1)	13(1)
C(20)	2877(3)	2053(2)	9298(1)	14(1)
C(21)	1563(3)	2754(2)	9310(1)	19(1)
C(22)	3750(3)	2299(2)	8695(1)	18(1)

Table 3. Selected bond lengths [Å] and angles [°] for CCDC 642801.

Ru(1)-C(13)	1.826(2)	C(13)-Ru(1)-C(1)	94.72(9)
Ru(1)-C(1)	1.947(2)	C(13)-Ru(1)-O(1)	79.56(8)
Ru(1)-O(1)	2.2699(16)	C(1)-Ru(1)-O(1)	173.94(7)
Ru(1)-Cl(2)	2.3265(6)	C(13)-Ru(1)-Cl(2)	101.61(7)
Ru(1)-Cl(1)	2.3533(5)	C(1)-Ru(1)-Cl(2)	92.51(7)
		O(1)-Ru(1)-Cl(2)	86.76(4)
		C(13)-Ru(1)-Cl(1)	100.86(7)
		C(1)-Ru(1)-Cl(1)	94.72(7)
		O(1)-Ru(1)-Cl(1)	88.35(4)
		Cl(2)-Ru(1)-Cl(1)	155.714(19)

Table 4. Bond lengths [Å] and angles [°] for CCDC 642801.

Ru(1)-C(13)	1.826(2)	C(21)-H(21B)	0.97(3)
Ru(1)-C(1)	1.947(2)	C(21)-H(21C)	1.00(3)
Ru(1)-O(1)	2.2699(16)	C(22)-H(22A)	1.00(4)
Ru(1)-Cl(2)	2.3265(6)	C(22)-H(22B)	0.99(3)
Ru(1)-Cl(1)	2.3533(5)	C(22)-H(22C)	0.96(3)
O(1)-C(19)	1.370(3)		
O(1)-C(20)	1.482(3)	C(13)-Ru(1)-C(1)	94.72(9)
N(1)-C(1)	1.363(3)	C(13)-Ru(1)-O(1)	79.56(8)
N(1)-C(2)	1.416(3)	C(1)-Ru(1)-O(1)	173.94(7)
N(1)-C(6)	1.450(3)	C(13)-Ru(1)-Cl(2)	101.61(7)
S(1)-C(1)	1.729(2)	C(1)-Ru(1)-Cl(2)	92.51(7)
S(1)-C(3)	1.738(2)	O(1)-Ru(1)-Cl(2)	86.76(4)
C(2)-C(3)	1.342(3)	C(13)-Ru(1)-Cl(1)	100.86(7)
C(2)-C(4)	1.501(3)	C(1)-Ru(1)-Cl(1)	94.72(7)
C(3)-C(5)	1.491(3)	O(1)-Ru(1)-Cl(1)	88.35(4)
C(4)-H(4A)	0.92(3)	Cl(2)-Ru(1)-Cl(1)	155.714(19)
C(4)-H(4B)	0.93(4)	C(19)-O(1)-C(20)	120.25(17)
C(4)-H(4C)	0.95(3)	C(19)-O(1)-Ru(1)	109.37(12)
C(5)-H(5A)	1.05(3)	C(20)-O(1)-Ru(1)	129.21(13)
C(5)-H(5B)	0.95(4)	C(1)-N(1)-C(2)	116.94(18)
C(5)-H(5C)	0.73(3)	C(1)-N(1)-C(6)	119.45(19)
C(6)-C(11)	1.389(3)	C(2)-N(1)-C(6)	123.6(2)
C(6)-C(7)	1.414(3)	C(1)-S(1)-C(3)	94.02(11)
C(7)-C(8)	1.382(3)	N(1)-C(1)-S(1)	106.85(16)
C(7)-H(7)	0.98(2)	N(1)-C(1)-Ru(1)	125.30(15)
C(8)-C(9)	1.389(4)	S(1)-C(1)-Ru(1)	127.84(12)
C(8)-H(8)	0.94(3)	C(3)-C(2)-N(1)	112.0(2)
C(9)-C(10)	1.370(4)	C(3)-C(2)-C(4)	127.9(2)
C(9)-H(9)	0.96(2)	N(1)-C(2)-C(4)	119.98(19)
C(10)-C(11)	1.410(3)	C(2)-C(3)-C(5)	128.4(2)
C(10)-H(10)	0.83(3)	C(2)-C(3)-S(1)	110.20(17)
C(11)-C(12)	1.491(4)	C(5)-C(3)-S(1)	121.39(18)
C(12)-H(12A)	0.94(3)	C(2)-C(4)-H(4A)	106.2(17)
C(12)-H(12B)	1.05(3)	C(2)-C(4)-H(4B)	112(2)
C(12)-H(12C)	0.91(3)	H(4A)-C(4)-H(4B)	113(3)
C(13)-C(14)	1.448(3)	C(2)-C(4)-H(4C)	123.6(18)
C(13)-H(13)	1.01(3)	H(4A)-C(4)-H(4C)	105(2)
C(14)-C(15)	1.394(3)	H(4B)-C(4)-H(4C)	97(3)
C(14)-C(19)	1.415(3)	C(3)-C(5)-H(5A)	106.2(15)
C(15)-C(16)	1.390(3)	C(3)-C(5)-H(5B)	105(2)
C(15)-H(15)	0.96(3)	H(5A)-C(5)-H(5B)	116(3)
C(16)-C(17)	1.399(3)	C(3)-C(5)-H(5C)	114(3)
C(16)-H(16)	0.96(2)	H(5A)-C(5)-H(5C)	116(3)
C(17)-C(18)	1.392(3)	H(5B)-C(5)-H(5C)	99(3)
C(17)-H(17)	1.02(3)	C(11)-C(6)-C(7)	122.2(2)
C(18)-C(19)	1.395(3)	C(11)-C(6)-N(1)	120.7(2)
C(18)-H(18)	0.90(3)	C(7)-C(6)-N(1)	117.1(2)
C(20)-C(21)	1.506(3)	C(8)-C(7)-C(6)	119.5(2)
C(20)-C(22)	1.508(3)	C(8)-C(7)-H(7)	120.7(14)
C(20)-H(20)	0.89(3)	C(6)-C(7)-H(7)	119.7(14)
C(21)-H(21A)	1.04(3)	C(7)-C(8)-C(9)	119.2(2)

C(7)-C(8)-H(8)	120.9(18)	H(22A)-C(22)-H(22C)	119(3)
C(9)-C(8)-H(8)	119.9(18)	H(22B)-C(22)-H(22C)	106(2)
C(10)-C(9)-C(8)	120.5(2)		
C(10)-C(9)-H(9)	118.8(15)		
C(8)-C(9)-H(9)	120.6(15)		
C(9)-C(10)-C(11)	122.6(2)		
C(9)-C(10)-H(10)	127(2)		
C(11)-C(10)-H(10)	111(2)		
C(6)-C(11)-C(10)	115.9(2)		
C(6)-C(11)-C(12)	123.3(2)		
C(10)-C(11)-C(12)	120.6(2)		
C(11)-C(12)-H(12A)	111.0(17)		
C(11)-C(12)-H(12B)	111.6(17)		
H(12A)-C(12)-H(12B)	98(2)		
C(11)-C(12)-H(12C)	117(2)		
H(12A)-C(12)-H(12C)	110(3)		
H(12B)-C(12)-H(12C)	108(2)		
C(14)-C(13)-Ru(1)	119.42(15)		
C(14)-C(13)-H(13)	116.4(15)		
Ru(1)-C(13)-H(13)	124.1(15)		
C(15)-C(14)-C(19)	118.5(2)		
C(15)-C(14)-C(13)	124.1(2)		
C(19)-C(14)-C(13)	117.42(19)		
C(16)-C(15)-C(14)	121.4(2)		
C(16)-C(15)-H(15)	116.9(16)		
C(14)-C(15)-H(15)	121.3(17)		
C(15)-C(16)-C(17)	119.0(2)		
C(15)-C(16)-H(16)	118.6(15)		
C(17)-C(16)-H(16)	122.4(15)		
C(18)-C(17)-C(16)	121.1(2)		
C(18)-C(17)-H(17)	121.5(15)		
C(16)-C(17)-H(17)	117.3(15)		
C(17)-C(18)-C(19)	119.2(2)		
C(17)-C(18)-H(18)	114.4(17)		
C(19)-C(18)-H(18)	126.2(17)		
O(1)-C(19)-C(18)	125.1(2)		
O(1)-C(19)-C(14)	114.20(18)		
C(18)-C(19)-C(14)	120.7(2)		
O(1)-C(20)-C(21)	105.31(19)		
O(1)-C(20)-C(22)	111.42(18)		
C(21)-C(20)-C(22)	113.3(2)		
O(1)-C(20)-H(20)	106.6(19)		
C(21)-C(20)-H(20)	117.0(19)		
C(22)-C(20)-H(20)	103.1(19)		
C(20)-C(21)-H(21A)	109.5(15)		
C(20)-C(21)-H(21B)	104(2)		
H(21A)-C(21)-H(21B)	109(2)		
C(20)-C(21)-H(21C)	107.7(14)		
H(21A)-C(21)-H(21C)	111(2)		
H(21B)-C(21)-H(21C)	116(2)		
C(20)-C(22)-H(22A)	112(2)		
C(20)-C(22)-H(22B)	108.5(18)		
H(22A)-C(22)-H(22B)	102(3)		
C(20)-C(22)-H(22C)	107.7(19)		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for CCDC 642801. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	88(1)	78(1)	105(1)	0(1)	-1(1)	-3(1)
Cl(1)	157(2)	138(2)	128(2)	-5(2)	16(2)	16(2)
Cl(2)	159(2)	155(2)	119(2)	16(2)	18(2)	-15(2)
O(1)	118(7)	85(6)	170(8)	-22(5)	-9(7)	-19(6)
N(1)	99(8)	129(8)	107(8)	18(6)	-10(7)	-4(7)
S(1)	125(2)	90(2)	209(3)	7(2)	-32(2)	-8(2)
C(1)	139(10)	104(9)	96(9)	13(7)	15(8)	19(8)
C(2)	119(10)	153(10)	113(10)	-23(8)	11(8)	-20(8)
C(3)	109(9)	161(10)	152(10)	-42(8)	-2(8)	-3(9)
C(4)	115(10)	204(10)	198(11)	-12(8)	-31(10)	-9(11)
C(5)	185(12)	159(11)	237(13)	-61(10)	1(11)	-15(10)
C(6)	104(10)	117(9)	154(11)	25(8)	-9(9)	-17(8)
C(7)	114(10)	148(9)	146(11)	41(7)	1(8)	14(8)
C(8)	228(12)	147(10)	179(11)	3(8)	16(10)	18(10)
C(9)	250(13)	113(10)	251(13)	41(9)	-10(11)	-4(10)
C(10)	247(12)	149(10)	182(11)	75(9)	14(10)	37(11)
C(11)	163(11)	177(10)	139(10)	25(8)	-10(9)	3(9)
C(12)	247(13)	215(12)	172(12)	14(10)	-22(11)	27(11)
C(13)	136(10)	103(8)	103(10)	-4(7)	7(8)	-16(8)
C(14)	118(10)	107(9)	113(9)	8(7)	11(8)	10(8)
C(15)	168(11)	119(9)	114(10)	15(7)	4(9)	36(9)
C(16)	146(11)	179(10)	143(10)	29(8)	-9(9)	31(9)
C(17)	125(11)	225(10)	174(11)	6(8)	-11(10)	0(10)
C(18)	151(10)	152(10)	168(9)	-16(8)	-35(8)	-22(11)
C(19)	127(8)	135(9)	117(8)	-10(9)	-2(7)	-2(10)
C(20)	140(11)	116(9)	169(11)	-39(8)	2(9)	-27(9)
C(21)	161(11)	117(10)	286(14)	-33(9)	38(10)	46(9)
C(22)	197(12)	157(11)	176(11)	6(9)	7(10)	-33(10)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CCDC 642801.

	x	y	z	U_{iso}
H(4A)	-5170(30)	-1380(20)	7803(14)	21(8)
H(4B)	-4440(40)	-320(30)	7470(20)	77(14)
H(4C)	-5160(30)	-160(30)	8076(16)	41(9)
H(5A)	-4830(30)	-3130(20)	8052(15)	24(8)
H(5B)	-3810(40)	-3860(30)	8595(19)	54(12)
H(5C)	-3530(30)	-3870(30)	7973(17)	33(10)
H(7)	-2510(20)	1170(20)	9279(12)	4(6)
H(8)	-2530(30)	3250(30)	9164(15)	28(8)
H(9)	-2220(20)	4110(20)	8113(12)	7(6)
H(10)	-2080(30)	2810(30)	7218(16)	31(9)
H(12A)	-1710(30)	-180(30)	7133(14)	27(8)
H(12B)	-1070(30)	850(30)	6773(16)	34(9)
H(12C)	-2660(30)	600(30)	6724(16)	39(10)
H(13)	1200(30)	-2200(20)	9014(15)	21(7)
H(15)	3550(30)	-2980(20)	9330(13)	15(7)
H(16)	5730(30)	-2680(20)	9723(12)	9(6)
H(17)	6580(30)	-740(20)	9938(13)	12(7)
H(18)	5090(30)	820(20)	9795(14)	12(7)
H(20)	3460(30)	2160(30)	9634(14)	21(8)
H(21A)	1000(30)	2580(20)	8883(14)	19(7)
H(21B)	1870(30)	3570(30)	9302(16)	41(10)
H(21C)	1040(30)	2510(20)	9716(12)	9(6)
H(22A)	4620(40)	1840(30)	8698(17)	53(11)
H(22B)	4080(30)	3130(30)	8719(15)	32(9)
H(22C)	3170(30)	2260(30)	8313(16)	28(8)

[$RuCl_2$ (3-(2,4,6-trimethylphenyl)-4,5-dimethylthiazol-2-ylidene) (=CH-*o*-*i*PrO-Ph)] (8)

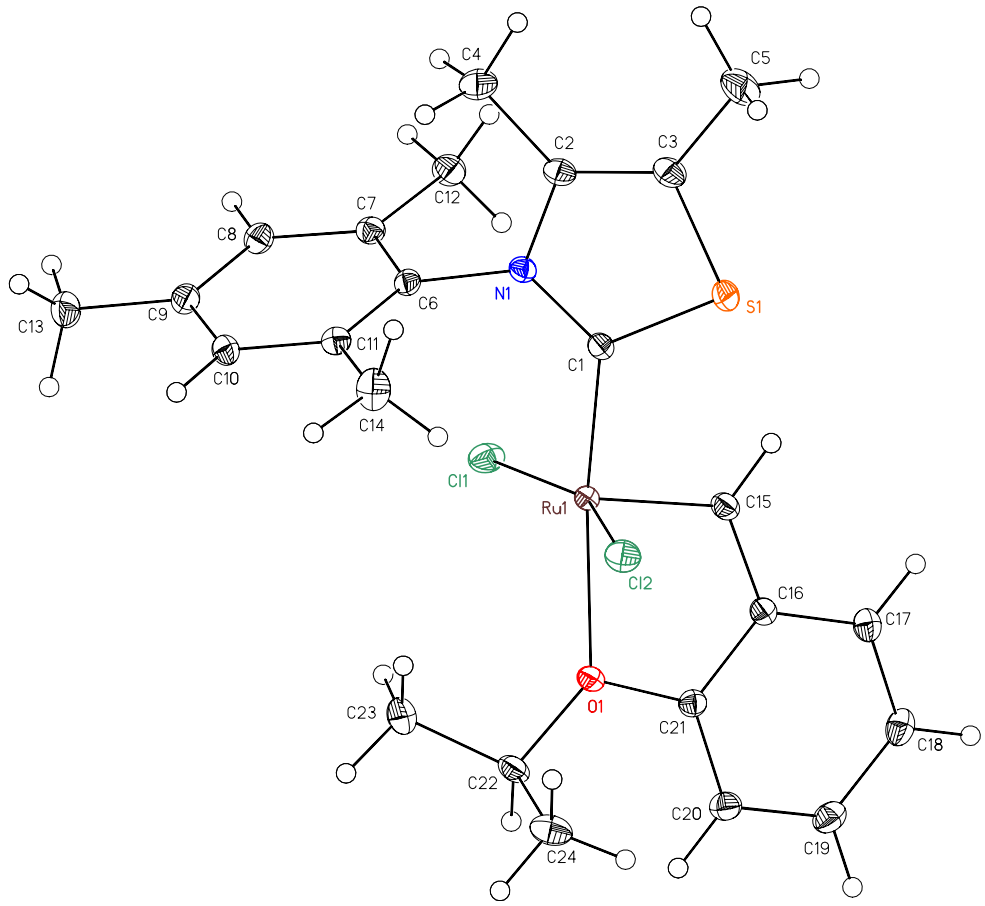


Table 1. Crystal data and structure refinement for CCDC 639435.

Empirical formula	$C_{24}H_{29}NOSCl_2Ru \bullet \frac{1}{2}(C_6H_6)$
Formula weight	590.57
Crystallization Solvent	Benzene/hexanes
Crystal Habit	Fragment
Crystal size	0.35 x 0.27 x 0.19 mm^3
Crystal color	Dark green

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 28680 reflections used in lattice determination	2.29 to 41.72°
Unit cell dimensions	a = 12.5506(4) Å b = 15.6147(4) Å β= 109.0050(10)° c = 14.3088(4) Å
Volume	2651.30(13) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.480 Mg/m^3
F(000)	1212
Data collection program	Bruker SMART v5.630
θ range for data collection	1.88 to 41.85°
Completeness to θ = 41.85°	96.0 %
Index ranges	$-23 \le h \le 21$, $-29 \le k \le 28$, $-26 \le l \le 26$
Data collection scan type	ω scans at 7 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	73622
Independent reflections	17644 [R_{int}= 0.0800]
Absorption coefficient	0.892 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8488 and 0.7455

Table 1 (cont.)

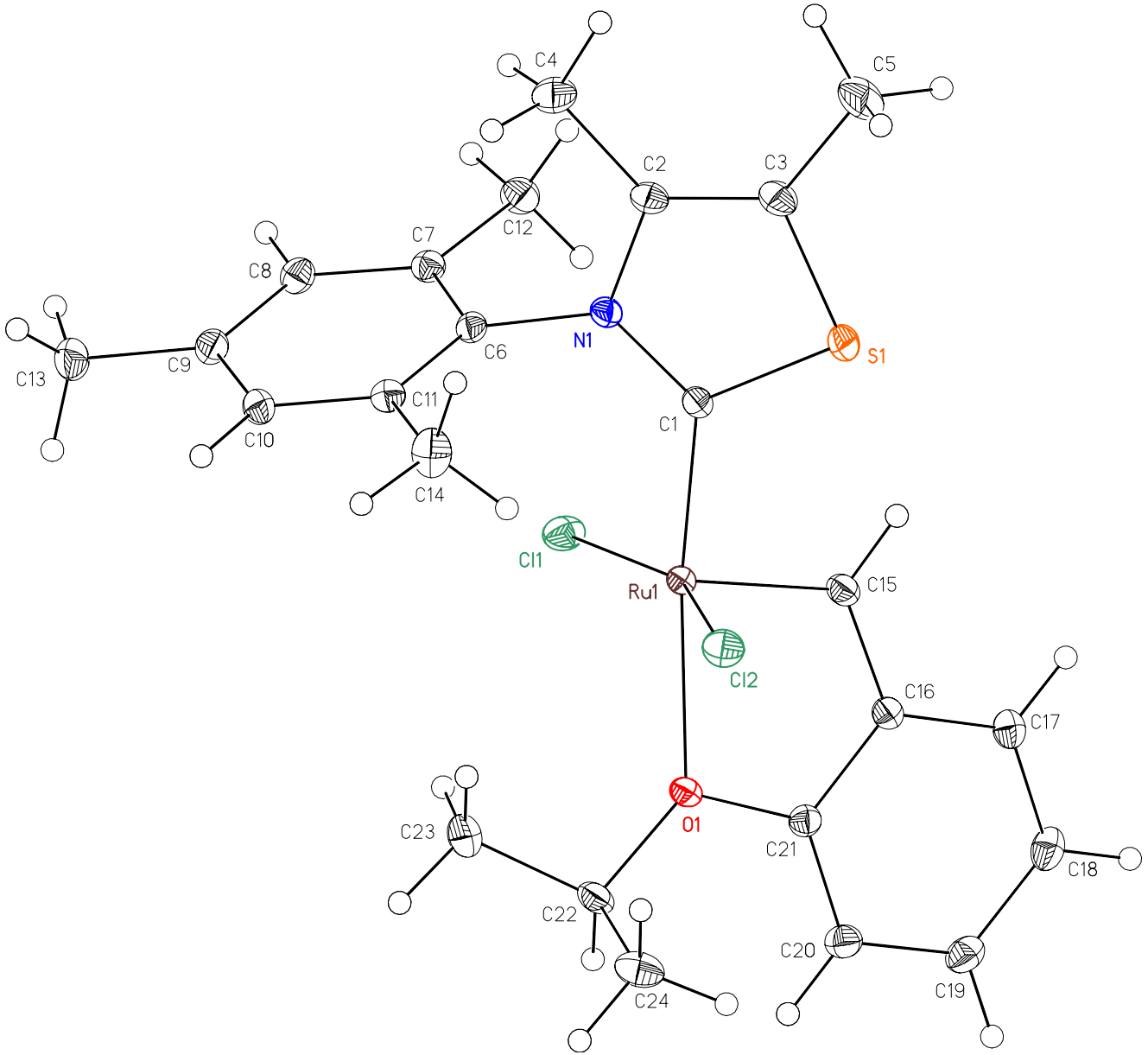
Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	17644 / 0 / 305
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.217
Final R indices [$I>2\sigma(I)$, 12744 reflections]	R1 = 0.0350, *w*R2 = 0.0674
R indices (all data)	R1 = 0.0563, *w*R2 = 0.0706
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.489 and -1.084 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C4
C5
C2
C3
C12
C7
C8
N1
C6
S1
C13
C9
C11
C1
C10
C14
Cl1
Ru1
C15
Cl2
C16
C17
O1
C23
C21
C18
C22
C20
C19
C24

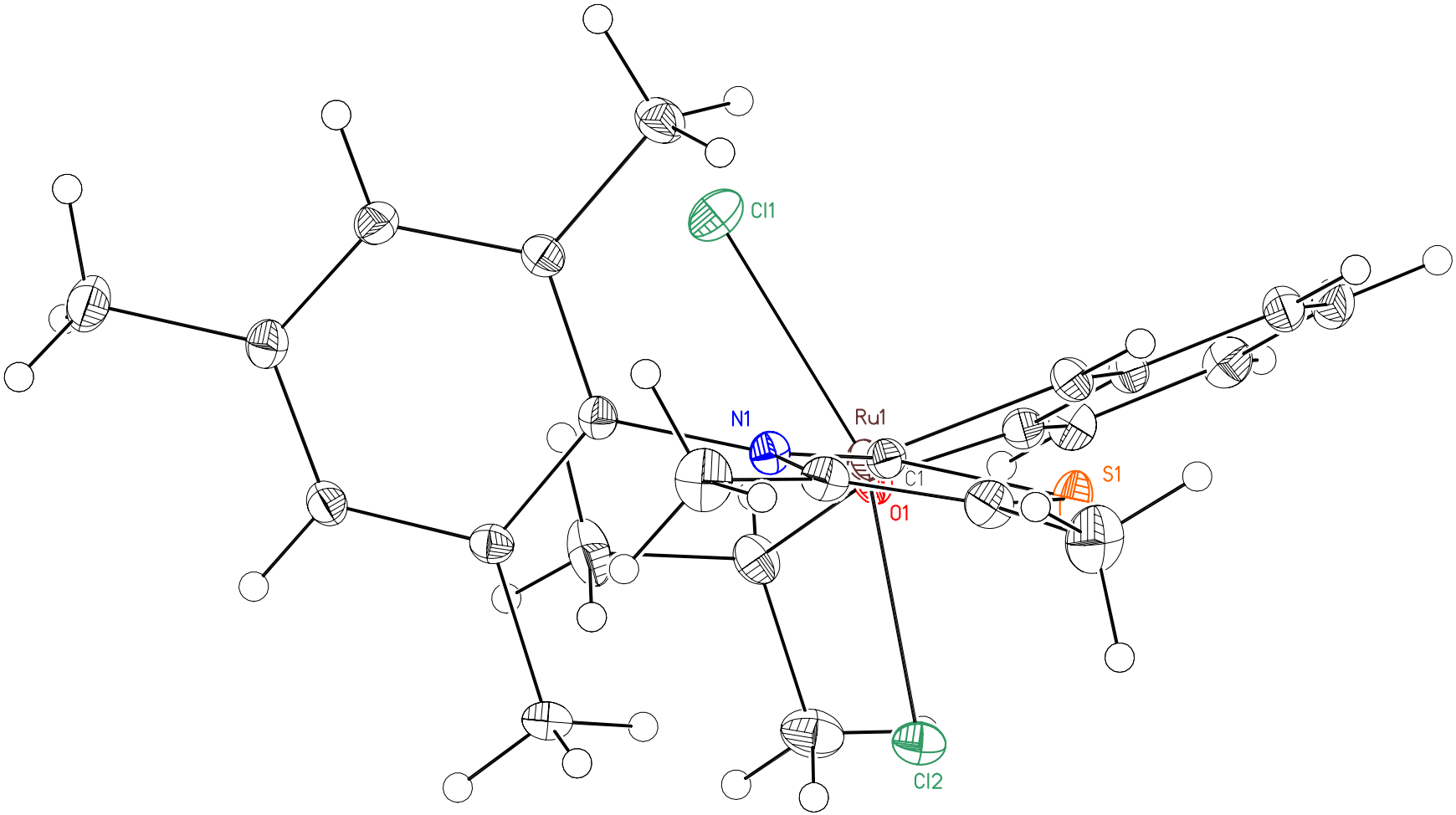

Cl1
N1
Ru1
C1
O1
S1
Cl2

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CCDC 639435. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	246(1)	2564(1)	1545(1)	10(1)
Cl(1)	-1041(1)	1730(1)	2015(1)	17(1)
Cl(2)	1927(1)	3269(1)	1663(1)	17(1)
S(1)	-615(1)	4454(1)	801(1)	15(1)
O(1)	1058(1)	1347(1)	1219(1)	13(1)
N(1)	-586(1)	4035(1)	2492(1)	11(1)
C(1)	-395(1)	3674(1)	1698(1)	11(1)
C(2)	-904(1)	4908(1)	2401(1)	13(1)
C(3)	-970(1)	5238(1)	1512(1)	15(1)
C(4)	-1097(1)	5364(1)	3255(1)	20(1)
C(5)	-1254(1)	6131(1)	1129(1)	24(1)
C(6)	-510(1)	3563(1)	3384(1)	11(1)
C(7)	-1515(1)	3260(1)	3490(1)	12(1)
C(8)	-1452(1)	2839(1)	4366(1)	14(1)
C(9)	-427(1)	2693(1)	5107(1)	14(1)
C(10)	557(1)	3001(1)	4969(1)	13(1)
C(11)	532(1)	3455(1)	4120(1)	12(1)
C(12)	-2626(1)	3361(1)	2679(1)	17(1)
C(13)	-378(1)	2209(1)	6031(1)	20(1)
C(14)	1604(1)	3841(1)	4045(1)	20(1)
C(15)	-409(1)	2507(1)	202(1)	13(1)
C(16)	-103(1)	1808(1)	-327(1)	12(1)
C(17)	-577(1)	1704(1)	-1353(1)	14(1)
C(18)	-260(1)	1025(1)	-1828(1)	17(1)
C(19)	545(1)	444(1)	-1280(1)	16(1)
C(20)	1032(1)	531(1)	-257(1)	15(1)
C(21)	697(1)	1206(1)	214(1)	12(1)
C(22)	1992(1)	831(1)	1863(1)	15(1)
C(23)	1952(1)	943(1)	2900(1)	23(1)
C(24)	3098(1)	1116(1)	1758(1)	20(1)
C(30)	140(1)	666(1)	4412(1)	25(1)
C(31)	1038(1)	391(1)	5203(1)	29(1)
C(32)	899(1)	-274(1)	5795(1)	27(1)

Table 3. Selected bond lengths [Å] and angles [°] for CCDC 639435.

Ru(1)-C(15)	1.8296(11)	C(15)-Ru(1)-C(1)	95.78(5)
Ru(1)-C(1)	1.9535(11)	C(15)-Ru(1)-O(1)	79.75(4)
Ru(1)-O(1)	2.2752(8)	C(1)-Ru(1)-O(1)	173.03(4)
Ru(1)-Cl(2)	2.3358(3)	C(15)-Ru(1)-Cl(2)	100.70(4)
Ru(1)-Cl(1)	2.3382(3)	C(1)-Ru(1)-Cl(2)	88.21(3)
		O(1)-Ru(1)-Cl(2)	87.39(2)
		C(15)-Ru(1)-Cl(1)	99.13(4)
		C(1)-Ru(1)-Cl(1)	96.54(3)
		O(1)-Ru(1)-Cl(1)	89.47(2)
		Cl(2)-Ru(1)-Cl(1)	159.026(12)

Table 4. Bond lengths [Å] and angles [°] for CCDC 639435.

Ru(1)-C(15)	1.8296(11)	C(1)-S(1)-C(3)	94.05(6)
Ru(1)-C(1)	1.9535(11)	C(21)-O(1)-C(22)	119.32(9)
Ru(1)-O(1)	2.2752(8)	C(21)-O(1)-Ru(1)	109.31(6)
Ru(1)-Cl(2)	2.3358(3)	C(22)-O(1)-Ru(1)	130.32(7)
Ru(1)-Cl(1)	2.3382(3)	C(1)-N(1)-C(2)	116.40(9)
S(1)-C(1)	1.7246(11)	C(1)-N(1)-C(6)	123.18(9)
S(1)-C(3)	1.7393(12)	C(2)-N(1)-C(6)	120.39(9)
O(1)-C(21)	1.3767(13)	N(1)-C(1)-S(1)	107.52(8)
O(1)-C(22)	1.4732(13)	N(1)-C(1)-Ru(1)	130.81(8)
N(1)-C(1)	1.3566(14)	S(1)-C(1)-Ru(1)	120.98(6)
N(1)-C(2)	1.4151(14)	C(3)-C(2)-N(1)	112.48(10)
N(1)-C(6)	1.4499(14)	C(3)-C(2)-C(4)	127.61(11)
C(2)-C(3)	1.3495(17)	N(1)-C(2)-C(4)	119.89(10)
C(2)-C(4)	1.5001(17)	C(2)-C(3)-C(5)	129.31(12)
C(3)-C(5)	1.4988(16)	C(2)-C(3)-S(1)	109.55(9)
C(6)-C(11)	1.3965(16)	C(5)-C(3)-S(1)	121.12(10)
C(6)-C(7)	1.4013(16)	C(11)-C(6)-C(7)	122.15(10)
C(7)-C(8)	1.3940(16)	C(11)-C(6)-N(1)	120.17(10)
C(7)-C(12)	1.5043(16)	C(7)-C(6)-N(1)	117.63(10)
C(8)-C(9)	1.3938(17)	C(8)-C(7)-C(6)	117.81(11)
C(9)-C(10)	1.3967(17)	C(8)-C(7)-C(12)	120.70(11)
C(9)-C(13)	1.5067(16)	C(6)-C(7)-C(12)	121.47(10)
C(10)-C(11)	1.3983(16)	C(7)-C(8)-C(9)	121.97(11)
C(11)-C(14)	1.5097(16)	C(8)-C(9)-C(10)	118.38(11)
C(15)-C(16)	1.4495(15)	C(8)-C(9)-C(13)	120.90(11)
C(16)-C(17)	1.4024(15)	C(10)-C(9)-C(13)	120.72(11)
C(16)-C(21)	1.4094(15)	C(9)-C(10)-C(11)	121.74(11)
C(17)-C(18)	1.3855(17)	C(6)-C(11)-C(10)	117.86(11)
C(18)-C(19)	1.3939(18)	C(6)-C(11)-C(14)	122.35(10)
C(19)-C(20)	1.3968(17)	C(10)-C(11)-C(14)	119.73(10)
C(20)-C(21)	1.3887(16)	C(16)-C(15)-Ru(1)	118.72(8)
C(22)-C(24)	1.5112(18)	C(17)-C(16)-C(21)	118.76(10)
C(22)-C(23)	1.5114(17)	C(17)-C(16)-C(15)	122.72(10)
C(30)-C(31)	1.381(2)	C(21)-C(16)-C(15)	118.52(10)
C(30)-C(32)#1	1.383(2)	C(18)-C(17)-C(16)	120.74(11)
C(31)-C(32)	1.386(2)	C(17)-C(18)-C(19)	119.54(11)
C(32)-C(30)#1	1.383(2)	C(18)-C(19)-C(20)	121.06(11)
		C(21)-C(20)-C(19)	118.99(11)
C(15)-Ru(1)-C(1)	95.78(5)	O(1)-C(21)-C(20)	125.45(10)
C(15)-Ru(1)-O(1)	79.75(4)	O(1)-C(21)-C(16)	113.62(10)
C(1)-Ru(1)-O(1)	173.03(4)	C(20)-C(21)-C(16)	120.90(10)
C(15)-Ru(1)-Cl(2)	100.70(4)	O(1)-C(22)-C(24)	110.27(10)
C(1)-Ru(1)-Cl(2)	88.21(3)	O(1)-C(22)-C(23)	106.07(10)
O(1)-Ru(1)-Cl(2)	87.39(2)	C(24)-C(22)-C(23)	112.89(11)
C(15)-Ru(1)-Cl(1)	99.13(4)	C(31)-C(30)-C(32)#1	119.93(14)
C(1)-Ru(1)-Cl(1)	96.54(3)	C(30)-C(31)-C(32)	120.18(15)
O(1)-Ru(1)-Cl(1)	89.47(2)	C(30)#1-C(32)-C(31)	119.89(14)
Cl(2)-Ru(1)-Cl(1)	159.026(12)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+1

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for CCDC 639435. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	103(1)	104(1)	96(1)	6(1)	28(1)	18(1)
Cl(1)	200(1)	118(1)	232(1)	9(1)	122(1)	6(1)
Cl(2)	118(1)	183(1)	190(1)	-4(1)	41(1)	-4(1)
S(1)	204(2)	125(1)	137(1)	37(1)	69(1)	26(1)
O(1)	135(4)	143(4)	110(3)	6(3)	24(3)	52(3)
N(1)	125(4)	91(4)	115(4)	4(3)	36(3)	9(3)
C(1)	105(5)	109(4)	114(4)	15(3)	32(3)	6(3)
C(2)	138(5)	99(4)	162(5)	-8(3)	41(4)	7(3)
C(3)	165(6)	104(5)	175(5)	7(4)	41(4)	7(4)
C(4)	277(7)	130(5)	216(6)	-35(4)	95(5)	32(4)
C(5)	324(8)	121(5)	276(7)	55(4)	91(6)	43(5)
C(6)	136(5)	95(4)	101(4)	-12(3)	40(4)	1(3)
C(7)	123(5)	118(4)	123(4)	-14(3)	34(4)	1(3)
C(8)	133(5)	156(5)	139(5)	-4(4)	57(4)	-12(4)
C(9)	168(6)	140(5)	127(4)	-1(3)	58(4)	4(4)
C(10)	129(5)	152(5)	112(4)	5(3)	24(4)	7(4)
C(11)	117(5)	113(4)	127(4)	-18(3)	35(4)	-12(3)
C(12)	119(5)	206(6)	162(5)	-3(4)	27(4)	15(4)
C(13)	204(6)	228(6)	170(5)	61(4)	87(5)	25(4)
C(14)	127(6)	267(6)	175(5)	10(4)	27(4)	-67(4)
C(15)	116(5)	130(5)	126(4)	11(3)	24(3)	20(4)
C(16)	120(5)	119(4)	115(4)	5(3)	33(4)	7(3)
C(17)	154(5)	148(5)	120(4)	5(3)	30(4)	-12(4)
C(18)	218(6)	162(5)	125(5)	-18(4)	63(4)	-39(4)
C(19)	198(6)	144(5)	169(5)	-29(4)	90(4)	-10(4)
C(20)	159(6)	138(5)	162(5)	-8(4)	63(4)	16(4)
C(21)	109(5)	135(5)	121(4)	2(3)	41(4)	4(3)
C(22)	134(5)	143(5)	153(5)	23(4)	18(4)	48(4)
C(23)	252(7)	274(7)	131(5)	33(4)	25(5)	79(5)
C(24)	134(6)	188(6)	269(6)	-5(4)	41(5)	28(4)
C(30)	319(8)	226(6)	243(6)	28(5)	151(6)	46(5)
C(31)	214(8)	321(8)	332(8)	-22(6)	85(6)	-29(6)
C(32)	254(8)	322(8)	202(6)	13(5)	36(5)	84(6)

[$RuCl_2$ (3-(2,6-diethylphenyl)-4,5-dimethylthiazol-2-ylidene) (=CH-*o*-*i*PrO-Ph)] (9)

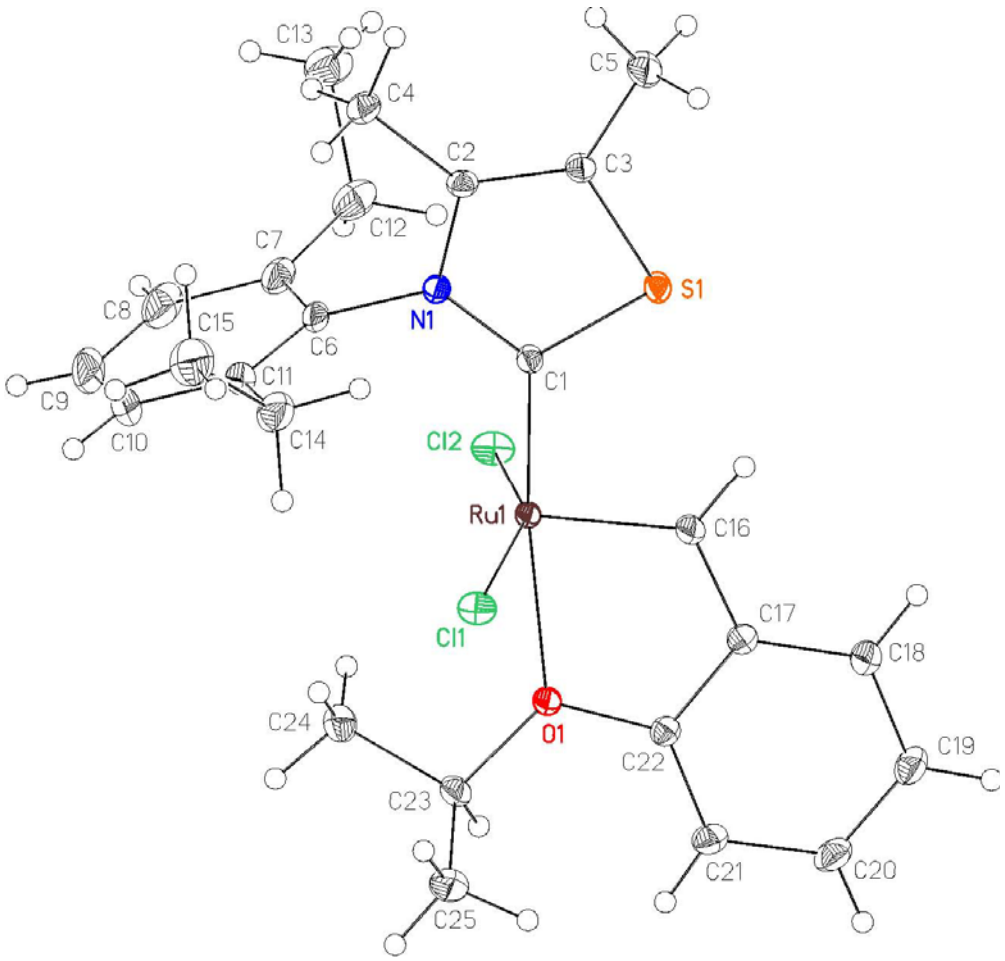


Table 1. Crystal data and structure refinement for CCDC 634944.

Empirical formula $C_{25}H_{31}NOSCl_2Ru$

Formula weight 565.54

Crystallization Solvent Benzene/Hexanes

Crystal Habit Fragment

Crystal size 0.34 x 0.31 x 0.29 mm^3

Crystal color Green/brown

Data Collection

Type of diffractometer Bruker SMART 1000

Wavelength 0.71073 Å MoKα

Data Collection Temperature 100(2) K

θ range for 33391 reflections used

in lattice determination 2.49 to 42.63°

Unit cell dimensions a = 16.2291(4) Å

b = 9.3934(2) Å β= 99.5100(10)°

c = 16.6087(4) Å

Volume 2497.14(10) $Å^3$

Z 4

Crystal system Monoclinic

Space group $P2_1/c$

Density (calculated) 1.504 Mg/m^3

F(000) 1160

Data collection program Bruker SMART v5.630

θ range for data collection 2.49 to 42.83°

Completeness to θ = 42.83° 94.3 %

Index ranges $-30 \leq h \leq 30$, $-17 \leq k \leq 17$, $-31 \leq l \leq 28$

Data collection scan type ω scans at 7 φ settings

Data reduction program Bruker SAINT v6.45A

Reflections collected 69940

Independent reflections 17254 [R_{int}= 0.0794]

Absorption coefficient 0.943 mm^{-1}

Absorption correction None

Max. and min. transmission 0.7716 and 0.7399

Table 1 (cont.)

Structure solution and Refinement

Structure solution program Bruker XS v6.12

Primary solution method Direct methods

Secondary solution method Difference Fourier map

Hydrogen placement Difference Fourier map

Structure refinement program Bruker XL v6.12

Refinement method Full matrix least-squares on F_2

Data / restraints / parameters 17254 / 0 / 404

Treatment of hydrogen atoms Unrestrained

Goodness-of-fit on F_2 1.261

Final R indices [$I>2\sigma(I)$, 13175 reflections] R1 = 0.0334, *w*R2 = 0.0666

R indices (all data) R1 = 0.0486, *w*R2 = 0.0690

Type of weighting scheme used Sigma

Weighting scheme used $w=1/\sigma_2(Fo_2)$

Max shift/error 0.004

Average shift/error 0.000

Largest diff. peak and hole 1.328 and -1.075 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

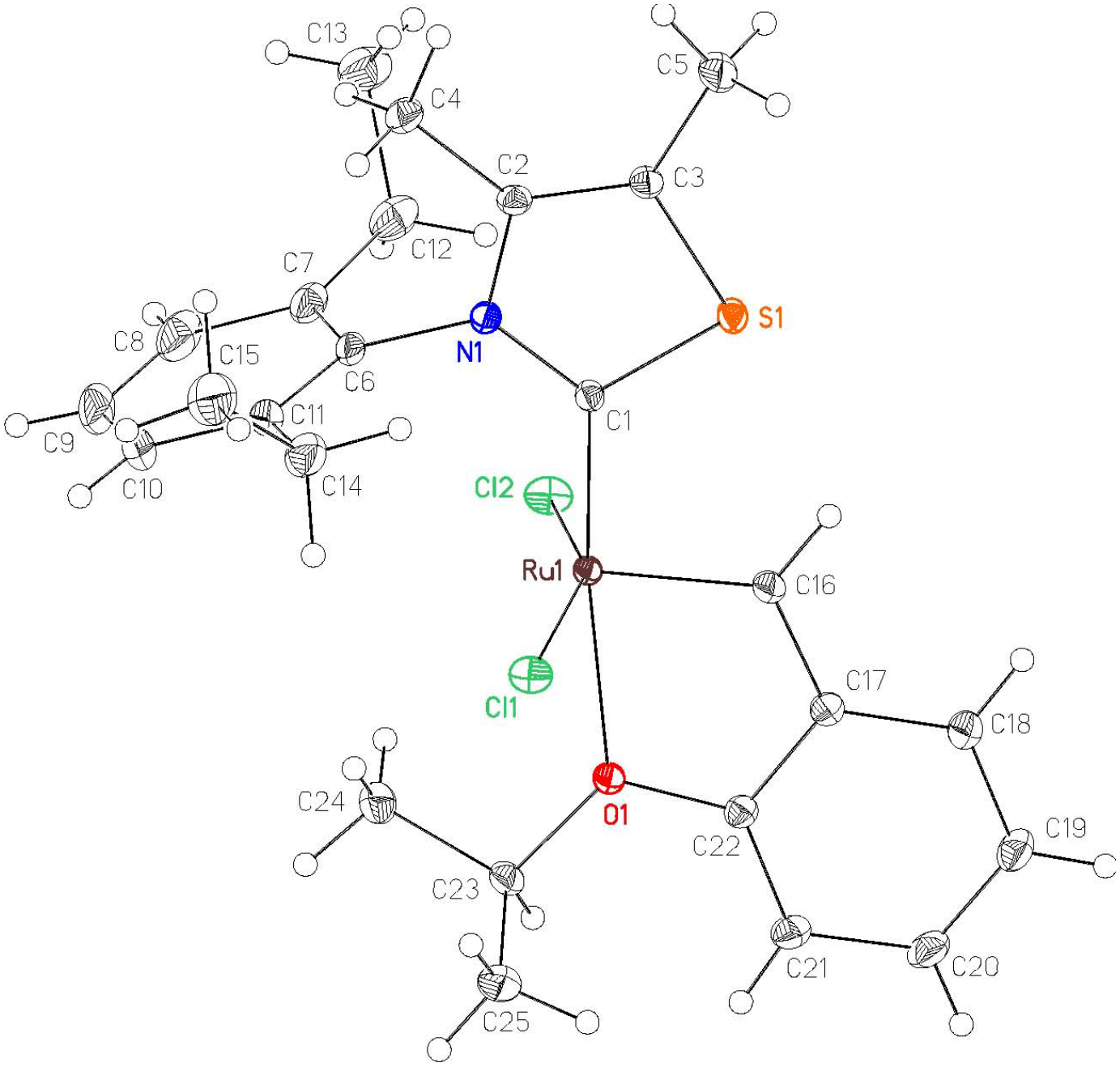

C13
C5
C4
C2
C3
C12
C7
S1
C8
C15
N1
C6
C1
C9
C11
C10
C14
Cl2
Ru1
C16
Cl1
C17
C18
C24
O1
C22
C19
C23
C21
C20
C25

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CCDC 634944. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	7295(1)	155(1)	6085(1)	9(1)
Cl(1)	7584(1)	-1245(1)	7255(1)	15(1)
Cl(2)	6653(1)	2019(1)	5298(1)	16(1)
S(1)	9233(1)	419(1)	5799(1)	12(1)
O(1)	6069(1)	-1047(1)	5816(1)	12(1)
N(1)	8727(1)	2018(1)	6811(1)	11(1)
C(1)	8414(1)	989(1)	6272(1)	10(1)
C(2)	9584(1)	2336(1)	6876(1)	12(1)
C(3)	9960(1)	1563(1)	6352(1)	12(1)
C(4)	9984(1)	3364(1)	7506(1)	16(1)
C(5)	10849(1)	1576(2)	6226(1)	20(1)
C(6)	8189(1)	2831(1)	7263(1)	14(1)
C(7)	7791(1)	4042(1)	6888(1)	18(1)
C(8)	7265(1)	4796(2)	7328(1)	27(1)
C(9)	7153(1)	4366(2)	8094(1)	32(1)
C(10)	7578(1)	3194(2)	8464(1)	26(1)
C(11)	8119(1)	2407(1)	8061(1)	19(1)
C(12)	7923(1)	4585(1)	6061(1)	22(1)
C(13)	8573(1)	5782(2)	6112(1)	26(1)
C(14)	8613(1)	1192(1)	8504(1)	23(1)
C(15)	9149(1)	1632(2)	9314(1)	31(1)
C(16)	7509(1)	-1050(1)	5277(1)	14(1)
C(17)	6874(1)	-2049(1)	4925(1)	13(1)
C(18)	6984(1)	-3009(1)	4303(1)	16(1)
C(19)	6355(1)	-3959(1)	3995(1)	19(1)
C(20)	5607(1)	-3941(1)	4299(1)	18(1)
C(21)	5473(1)	-2995(1)	4913(1)	15(1)
C(22)	6109(1)	-2053(1)	5223(1)	12(1)
C(23)	5324(1)	-980(1)	6219(1)	14(1)
C(24)	5375(1)	429(1)	6665(1)	18(1)
C(25)	5314(1)	-2237(1)	6796(1)	21(1)

Table 3. Selected bond lengths [Å] and angles [°] for CCDC 634944.

Ru(1)-C(16) 1.8321(11)
Ru(1)-C(1) 1.9546(10)
Ru(1)-O(1) 2.2680(7)
Ru(1)-Cl(2) 2.3262(3)
Ru(1)-Cl(1) 2.3292(3)

C(16)-Ru(1)-C(1) 94.63(4)
C(16)-Ru(1)-O(1) 79.30(4)
C(1)-Ru(1)-O(1) 173.18(3)
C(16)-Ru(1)-Cl(2) 100.11(4)
C(1)-Ru(1)-Cl(2) 96.10(3)
O(1)-Ru(1)-Cl(2) 88.09(2)
C(16)-Ru(1)-Cl(1) 103.02(4)
C(1)-Ru(1)-Cl(1) 92.30(3)
O(1)-Ru(1)-Cl(1) 86.10(2)
Cl(2)-Ru(1)-Cl(1) 154.632(11)

Table 4. Bond lengths [Å] and angles [°] for CCDC 634944.

Ru(1)-C(16)	1.8321(11)
Ru(1)-C(1)	1.9546(10)
Ru(1)-O(1)	2.2680(7)
Ru(1)-Cl(2)	2.3262(3)
Ru(1)-Cl(1)	2.3292(3)
S(1)-C(1)	1.7362(10)
S(1)-C(3)	1.7410(11)
O(1)-C(22)	1.3745(13)
O(1)-C(23)	1.4774(12)
N(1)-C(1)	1.3573(13)
N(1)-C(2)	1.4102(13)
N(1)-C(6)	1.4575(13)
C(2)-C(3)	1.3531(14)
C(2)-C(4)	1.4911(15)
C(3)-C(5)	1.4921(15)
C(4)-H(4A)	0.933(18)
C(4)-H(4B)	0.966(19)
C(4)-H(4C)	0.966(19)
C(5)-H(5A)	0.871(19)
C(5)-H(5B)	0.917(17)
C(5)-H(5C)	0.95(2)
C(6)-C(7)	1.4012(17)
C(6)-C(11)	1.4067(17)
C(7)-C(8)	1.4038(17)
C(7)-C(12)	1.513(2)
C(8)-C(9)	1.375(3)
C(8)-H(8)	0.88(2)
C(9)-C(10)	1.387(2)
C(9)-H(9)	0.88(2)
C(10)-C(11)	1.3995(17)
C(10)-H(10)	0.93(2)
C(11)-C(14)	1.514(2)
C(12)-C(13)	1.5352(19)
C(12)-H(12A)	0.98(2)
C(12)-H(12B)	0.943(15)
C(13)-H(13A)	0.911(17)
C(13)-H(13B)	0.942(18)
C(13)-H(13C)	0.90(2)
C(14)-C(15)	1.534(2)
C(14)-H(14A)	1.007(17)
C(14)-H(14B)	1.020(18)
C(15)-H(15A)	0.99(2)
C(15)-H(15B)	1.03(2)
C(15)-H(15C)	0.93(2)
C(16)-C(17)	1.4446(15)
C(16)-H(16)	0.968(17)
C(17)-C(18)	1.4052(15)
C(17)-C(22)	1.4105(14)
C(18)-C(19)	1.3874(16)

C(18)-H(18) 0.938(16)
C(19)-C(20) 1.3899(18)
C(19)-H(19) 0.921(18)
C(20)-C(21) 1.3967(17)
C(20)-H(20) 0.872(19)
C(21)-C(22) 1.3909(15)
C(21)-H(21) 0.916(15)
C(23)-C(24) 1.5114(16)
C(23)-C(25) 1.5222(17)
C(23)-H(23) 0.958(17)
C(24)-H(24A) 0.869(19)
C(24)-H(24B) 0.999(19)
C(24)-H(24C) 0.933(18)
C(25)-H(25A) 0.988(17)
C(25)-H(25B) 0.92(2)
C(25)-H(25C) 0.941(19)
C(16)-Ru(1)-C(1) 94.63(4)
C(16)-Ru(1)-O(1) 79.30(4)
C(1)-Ru(1)-O(1) 173.18(3)
C(16)-Ru(1)-Cl(2) 100.11(4)
C(1)-Ru(1)-Cl(2) 96.10(3)
O(1)-Ru(1)-Cl(2) 88.09(2)
C(16)-Ru(1)-Cl(1) 103.02(4)
C(1)-Ru(1)-Cl(1) 92.30(3)
O(1)-Ru(1)-Cl(1) 86.10(2)
Cl(2)-Ru(1)-Cl(1) 154.632(11)
C(1)-S(1)-C(3) 94.22(5)
C(22)-O(1)-C(23) 119.56(8)
C(22)-O(1)-Ru(1) 109.86(6)
C(23)-O(1)-Ru(1) 130.32(6)
C(1)-N(1)-C(2) 117.25(8)
C(1)-N(1)-C(6) 121.45(9)
C(2)-N(1)-C(6) 121.16(8)
N(1)-C(1)-S(1) 106.70(7)
N(1)-C(1)-Ru(1) 128.80(7)
S(1)-C(1)-Ru(1) 124.37(6)
C(3)-C(2)-N(1) 112.38(9)
C(3)-C(2)-C(4) 127.52(10)
N(1)-C(2)-C(4) 120.01(9)
C(2)-C(3)-C(5) 129.36(10)
C(2)-C(3)-S(1) 109.42(8)
C(5)-C(3)-S(1) 121.20(8)
C(2)-C(4)-H(4A) 107.8(11)
C(2)-C(4)-H(4B) 108.0(11)
H(4A)-C(4)-H(4B) 109.5(15)
C(2)-C(4)-H(4C) 111.0(11)
H(4A)-C(4)-H(4C) 108.2(15)
H(4B)-C(4)-H(4C) 112.3(15)
C(3)-C(5)-H(5A) 111.9(12)
C(3)-C(5)-H(5B) 109.2(11)
H(5A)-C(5)-H(5B) 103.0(16)
C(3)-C(5)-H(5C) 111.4(12)
H(5A)-C(5)-H(5C) 111.6(17)
H(5B)-C(5)-H(5C) 109.3(15)
C(7)-C(6)-C(11) 123.03(10)
C(7)-C(6)-N(1) 117.92(10)

C(11)-C(6)-N(1) 118.99(10)
C(6)-C(7)-C(8) 116.97(13)
C(6)-C(7)-C(12) 123.56(10)
C(8)-C(7)-C(12) 119.44(12)
C(9)-C(8)-C(7) 121.21(14)
C(9)-C(8)-H(8) 120.8(12)
C(7)-C(8)-H(8) 117.8(12)
C(8)-C(9)-C(10) 120.66(12)
C(8)-C(9)-H(9) 116.5(15)
C(10)-C(9)-H(9) 122.8(15)
C(9)-C(10)-C(11) 120.88(14)
C(9)-C(10)-H(10) 117.8(13)
C(11)-C(10)-H(10) 121.4(13)
C(10)-C(11)-C(6) 117.09(13)
C(10)-C(11)-C(14) 119.30(12)
C(6)-C(11)-C(14) 123.58(10)
C(7)-C(12)-C(13) 113.39(12)
C(7)-C(12)-H(12A) 109.0(12)
C(13)-C(12)-H(12A) 109.9(11)
C(7)-C(12)-H(12B) 111.9(9)
C(13)-C(12)-H(12B) 110.5(9)
H(12A)-C(12)-H(12B) 101.5(14)
C(12)-C(13)-H(13A) 110.6(11)
C(12)-C(13)-H(13B) 111.4(11)
H(13A)-C(13)-H(13B) 106.9(15)
C(12)-C(13)-H(13C) 111.4(12)
H(13A)-C(13)-H(13C) 110.3(16)
H(13B)-C(13)-H(13C) 106.0(16)
C(11)-C(14)-C(15) 113.65(12)
C(11)-C(14)-H(14A) 113.0(10)
C(15)-C(14)-H(14A) 108.7(10)
C(11)-C(14)-H(14B) 109.6(11)
C(15)-C(14)-H(14B) 111.0(10)
H(14A)-C(14)-H(14B) 100.0(14)
C(14)-C(15)-H(15A) 112.7(11)
C(14)-C(15)-H(15B) 112.3(11)
H(15A)-C(15)-H(15B) 110.2(16)
C(14)-C(15)-H(15C) 109.8(13)
H(15A)-C(15)-H(15C) 105.0(16)
H(15B)-C(15)-H(15C) 106.3(15)
C(17)-C(16)-Ru(1) 119.28(8)
C(17)-C(16)-H(16) 117.1(10)
Ru(1)-C(16)-H(16) 123.4(10)
C(18)-C(17)-C(22) 118.84(10)
C(18)-C(17)-C(16) 123.09(10)
C(22)-C(17)-C(16) 118.07(9)
C(19)-C(18)-C(17) 120.57(11)
C(19)-C(18)-H(18) 120.8(9)
C(17)-C(18)-H(18) 118.5(9)
C(18)-C(19)-C(20) 119.44(11)
C(18)-C(19)-H(19) 122.6(11)
C(20)-C(19)-H(19) 117.9(11)
C(19)-C(20)-C(21) 121.60(11)
C(19)-C(20)-H(20) 118.6(12)
C(21)-C(20)-H(20) 119.8(12)
C(22)-C(21)-C(20) 118.62(10)

C(22)-C(21)-H(21) 125.6(10)
C(20)-C(21)-H(21) 115.8(10)
O(1)-C(22)-C(21) 125.60(9)
O(1)-C(22)-C(17) 113.46(9)
C(21)-C(22)-C(17) 120.94(10)
O(1)-C(23)-C(24) 106.06(9)
O(1)-C(23)-C(25) 110.24(9)
C(24)-C(23)-C(25) 112.12(10)
O(1)-C(23)-H(23) 106.6(9)
C(24)-C(23)-H(23) 110.9(10)
C(25)-C(23)-H(23) 110.7(10)
C(23)-C(24)-H(24A) 110.6(11)
C(23)-C(24)-H(24B) 110.0(11)
H(24A)-C(24)-H(24B) 107.4(16)
C(23)-C(24)-H(24C) 110.4(11)
H(24A)-C(24)-H(24C) 112.5(16)
H(24B)-C(24)-H(24C) 105.8(15)
C(23)-C(25)-H(25A) 112.1(10)
C(23)-C(25)-H(25B) 112.1(12)
H(25A)-C(25)-H(25B) 110.1(15)
C(23)-C(25)-H(25C) 110.6(11)
H(25A)-C(25)-H(25C) 105.2(15)
H(25B)-C(25)-H(25C) 106.4(16)

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for CCDC 634944. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

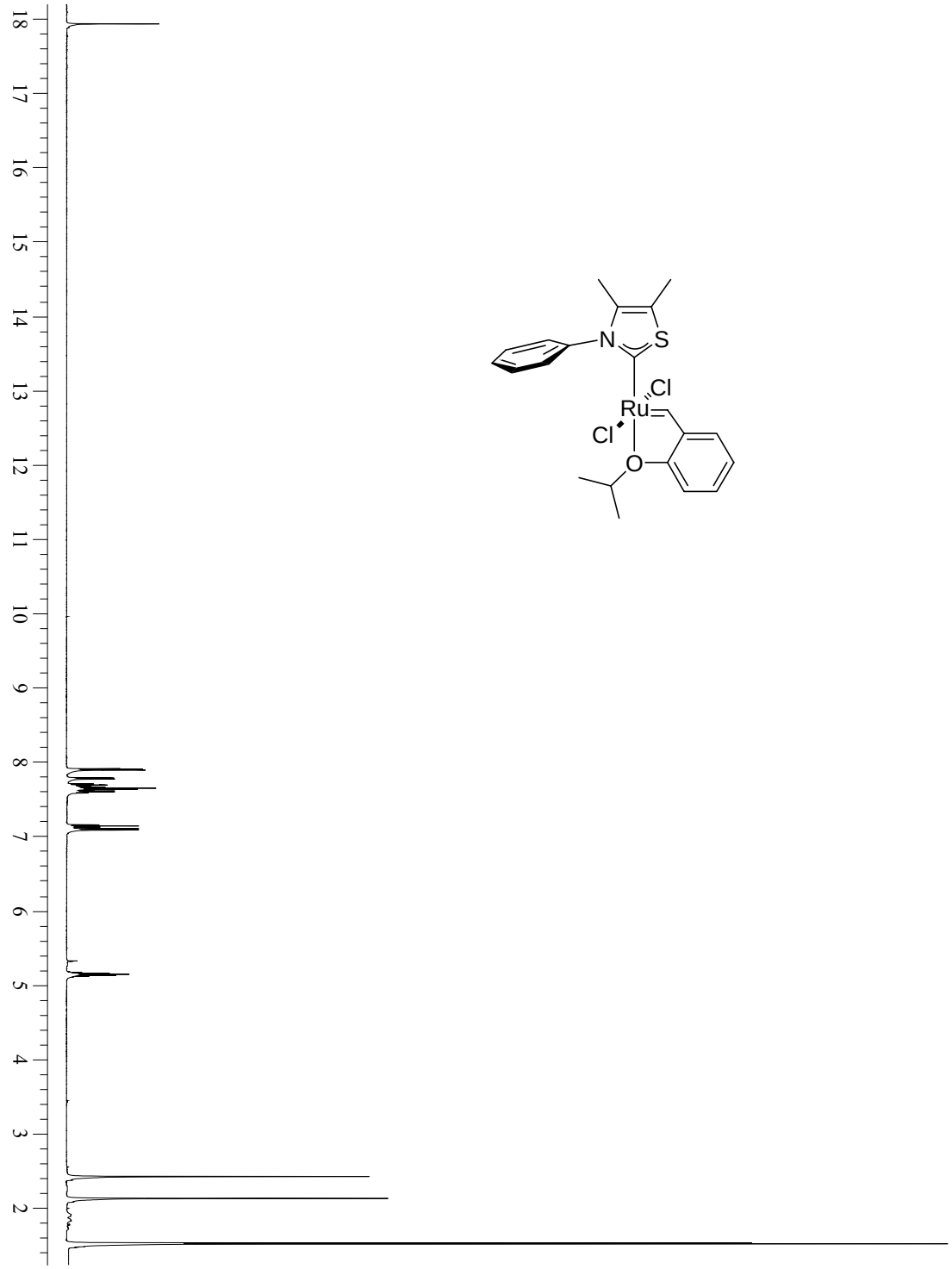
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	76(1)	99(1)	95(1)	-13(1)	19(1)	-6(1)
Cl(1)	138(1)	156(1)	148(1)	32(1)	5(1)	-6(1)
Cl(2)	130(1)	167(1)	188(1)	49(1)	-1(1)	0(1)
S(1)	91(1)	151(1)	125(1)	-42(1)	25(1)	-6(1)
O(1)	96(3)	137(3)	138(3)	-37(3)	36(3)	-23(2)
N(1)	93(3)	117(3)	130(4)	-30(3)	26(3)	-9(3)
C(1)	93(3)	108(4)	99(4)	-7(3)	19(3)	3(3)
C(2)	91(4)	121(4)	138(4)	-4(3)	16(3)	-14(3)
C(3)	88(4)	147(4)	126(4)	-18(3)	14(3)	-13(3)
C(4)	133(4)	170(5)	188(5)	-52(4)	21(4)	-37(3)
C(5)	101(4)	268(6)	233(6)	-86(5)	46(4)	-31(4)
C(6)	106(4)	139(4)	184(5)	-66(4)	51(4)	-19(3)
C(7)	123(4)	154(5)	265(6)	-77(4)	25(4)	2(3)
C(8)	156(5)	210(5)	440(8)	-125(6)	36(5)	34(4)
C(9)	183(5)	327(7)	470(9)	-219(7)	161(6)	-18(5)
C(10)	243(6)	305(7)	284(7)	-136(5)	160(6)	-74(5)
C(11)	195(5)	194(5)	192(5)	-73(4)	86(4)	-61(4)
C(12)	219(5)	145(5)	290(7)	-9(4)	-8(5)	7(4)
C(13)	221(6)	190(6)	364(8)	11(5)	33(6)	-4(4)
C(14)	331(7)	206(6)	169(5)	-33(4)	66(5)	-65(5)
C(15)	411(9)	345(8)	168(6)	-33(5)	51(6)	-85(6)
C(16)	111(4)	166(4)	140(5)	-38(3)	41(4)	-32(3)
C(17)	125(4)	141(4)	128(4)	-20(3)	20(4)	-21(3)
C(18)	170(5)	179(5)	149(5)	-43(4)	37(4)	-26(4)
C(19)	236(5)	177(5)	152(5)	-57(4)	20(4)	-38(4)
C(20)	194(5)	169(5)	175(5)	-40(4)	-4(4)	-64(4)
C(21)	134(4)	150(4)	170(5)	-13(4)	12(4)	-32(3)
C(22)	115(4)	123(4)	113(4)	-8(3)	10(3)	-11(3)
C(23)	101(4)	167(4)	149(5)	-15(4)	39(4)	-9(3)
C(24)	179(5)	169(5)	203(6)	-15(4)	67(5)	19(4)
C(25)	249(6)	186(5)	198(6)	10(4)	84(5)	-53(4)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CCDC 634944

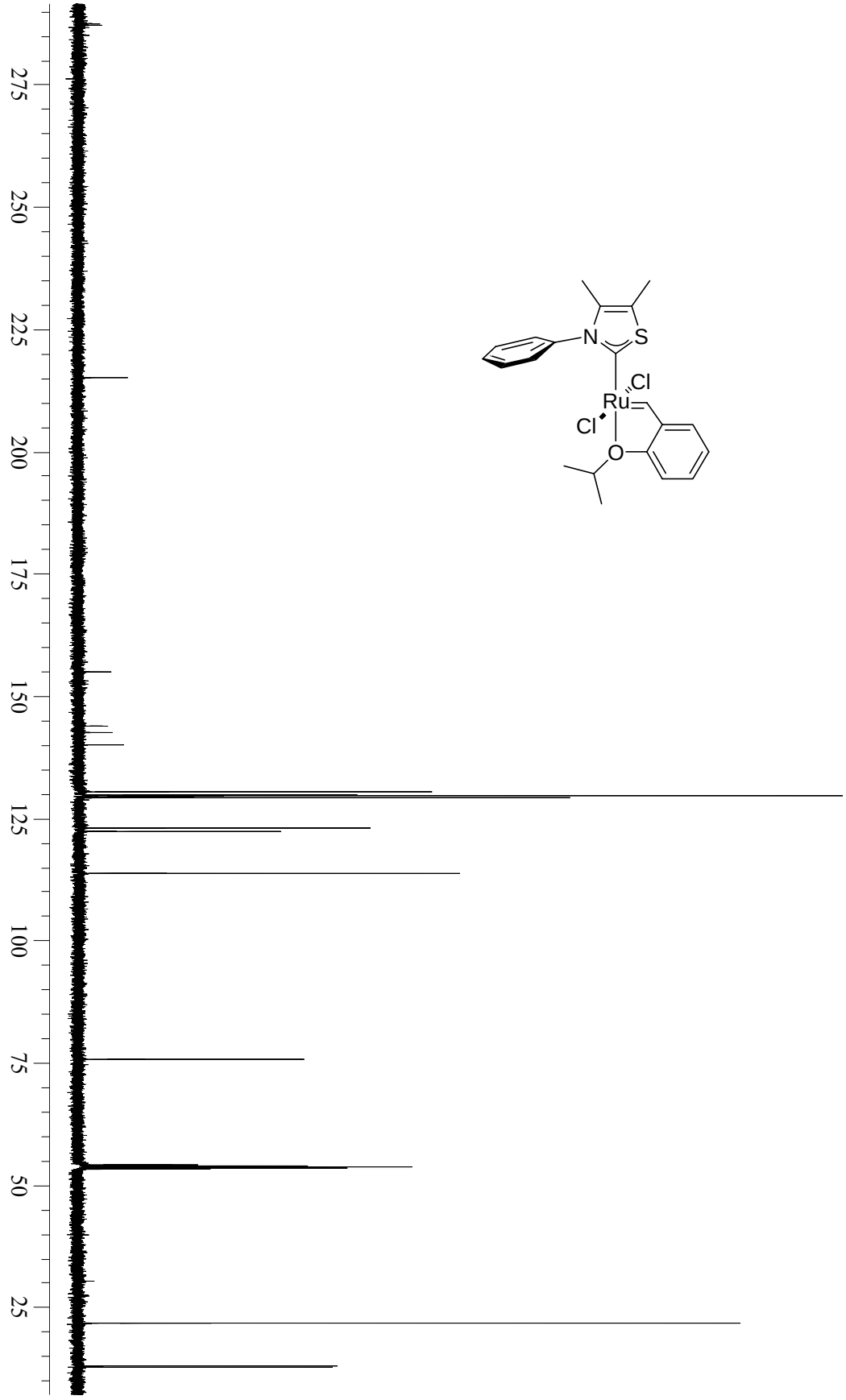
	x	y	z	U_{iso}
H(4A)	9956(11)	2980(20)	8018(11)	32(5)
H(4B)	9669(11)	4240(20)	7438(11)	27(4)
H(4C)	10566(12)	3510(20)	7466(11)	34(5)
H(5A)	11152(12)	2160(20)	6558(11)	31(5)
H(5B)	10878(11)	1953(17)	5722(10)	20(4)
H(5C)	11079(13)	650(20)	6260(12)	39(5)
H(8)	6976(12)	5510(20)	7082(12)	34(5)
H(9)	6818(16)	4890(20)	8337(14)	49(7)
H(10)	7490(13)	2950(20)	8983(12)	45(6)
H(12A)	7387(13)	4915(18)	5759(13)	33(5)
H(12B)	8056(10)	3843(17)	5722(9)	14(4)
H(13A)	8435(11)	6515(19)	6423(10)	22(4)
H(13B)	8604(11)	6159(19)	5592(11)	29(5)
H(13C)	9089(13)	5460(20)	6310(12)	34(5)
H(14A)	8980(11)	692(19)	8160(10)	26(4)
H(14B)	8218(12)	381(18)	8589(11)	24(4)
H(15A)	9546(12)	2400(20)	9248(11)	38(5)
H(15B)	9460(13)	780(20)	9617(12)	38(5)
H(15C)	8811(13)	2000(20)	9662(12)	37(5)
H(16)	8017(11)	-1017(18)	5043(10)	26(4)
H(18)	7481(10)	-2967(16)	4086(9)	15(4)
H(19)	6402(11)	-4582(19)	3577(11)	25(4)
H(20)	5216(12)	-4540(20)	4099(11)	30(5)
H(21)	4961(10)	-3049(18)	5074(9)	18(4)
H(23)	4847(10)	-1006(18)	5793(10)	19(4)
H(24A)	5803(12)	443(18)	7055(11)	22(4)
H(24B)	4864(12)	570(20)	6920(11)	33(5)
H(24C)	5380(11)	1179(19)	6298(11)	29(5)
H(25A)	5375(11)	-3156(18)	6522(10)	24(4)
H(25B)	4840(13)	-2250(20)	7037(12)	39(5)
H(25C)	5771(12)	-2192(19)	7224(11)	30(5)

NMR Spectra

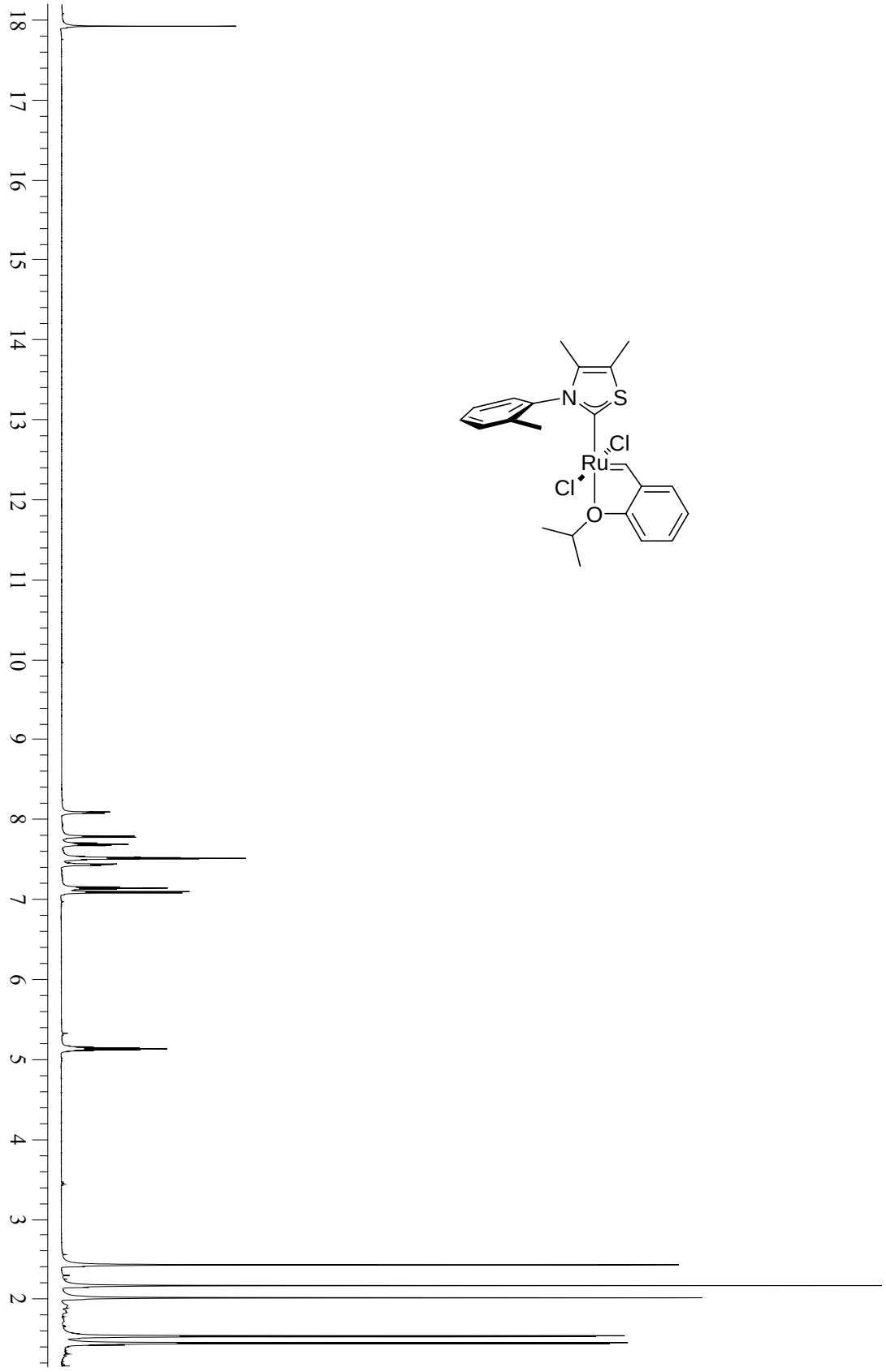
^{1}H NMR (CD_2Cl_2)



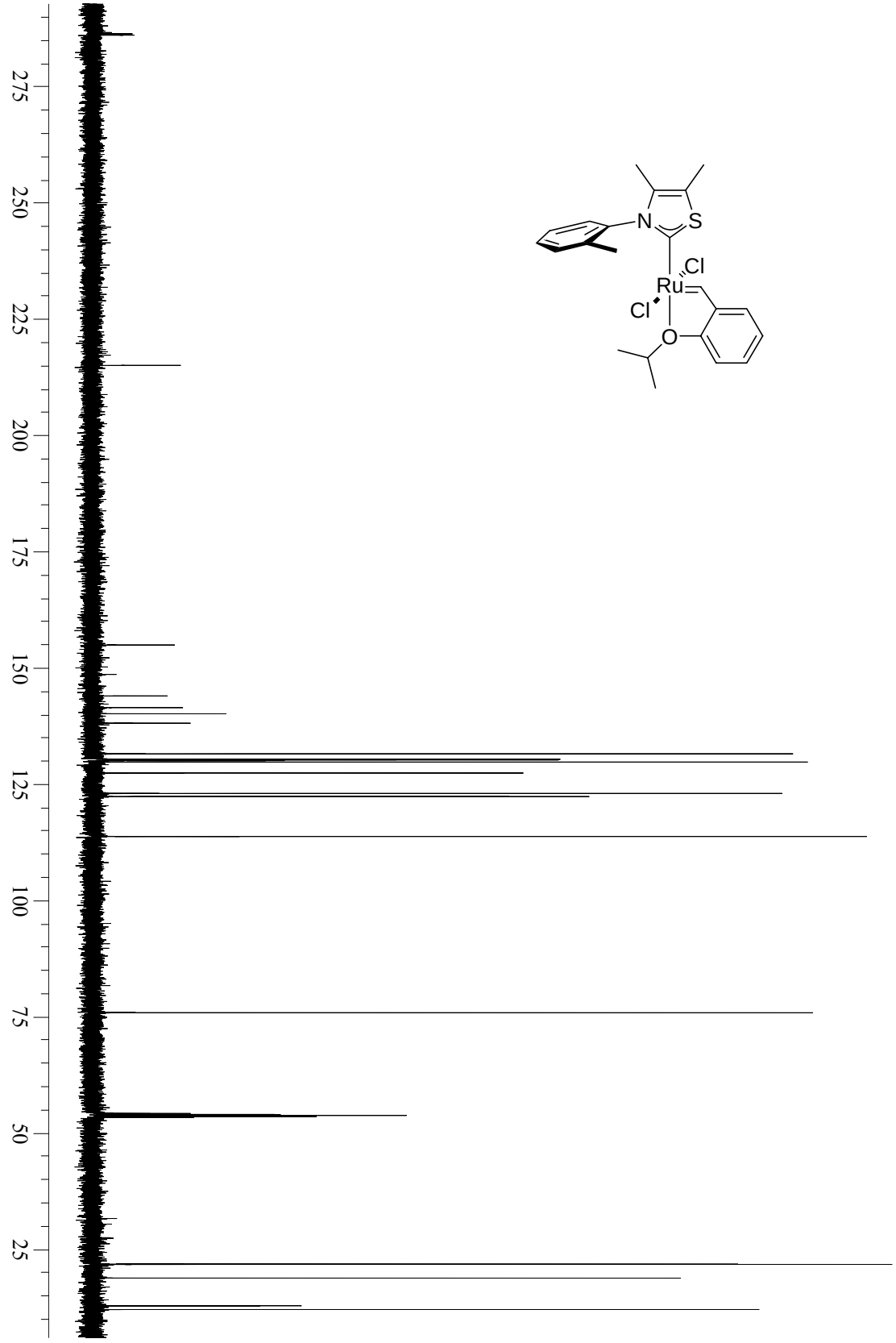
^{13}C NMR (CD_2Cl_2)



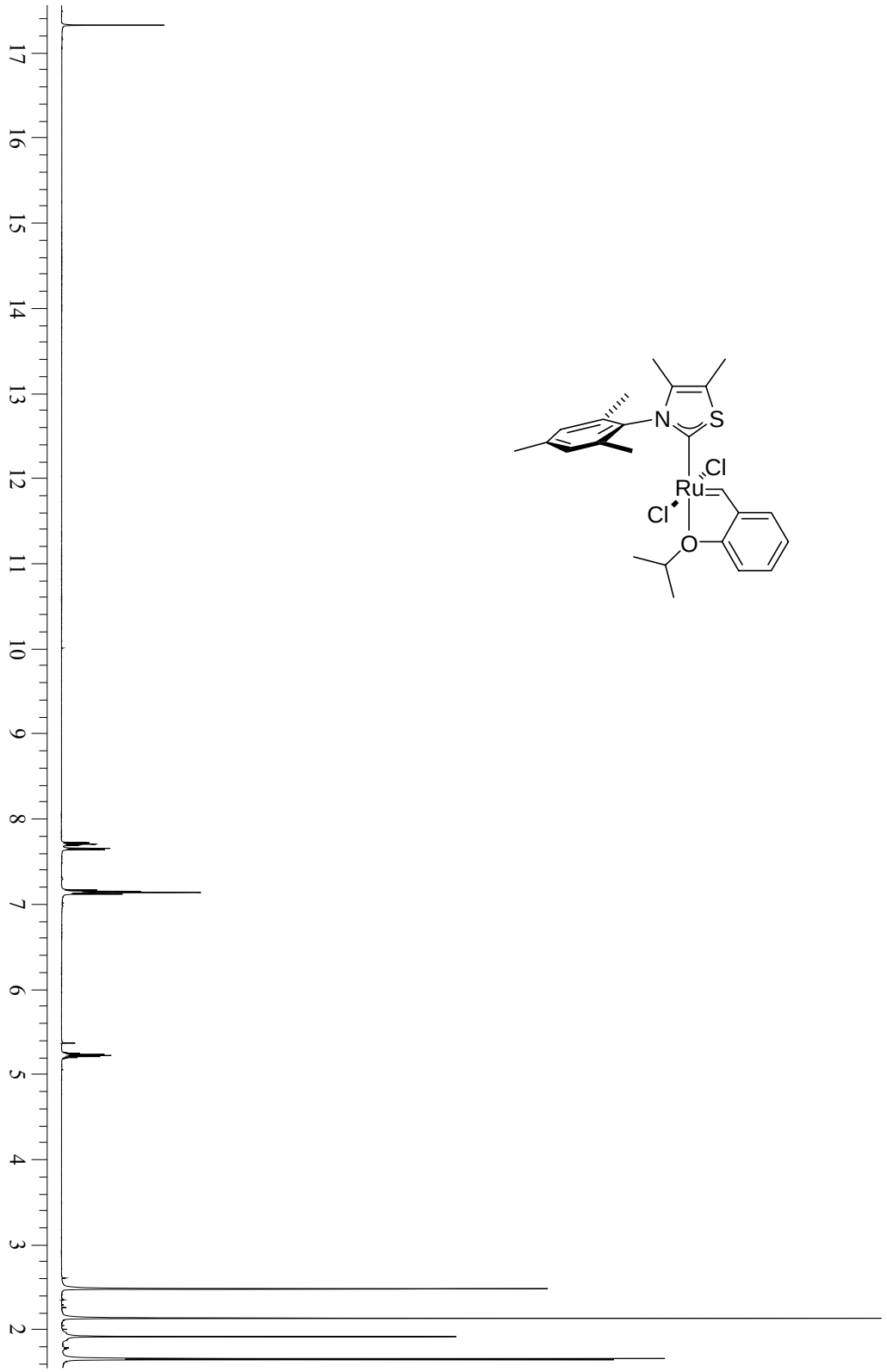
^{1}H NMR (CD_2Cl_2)



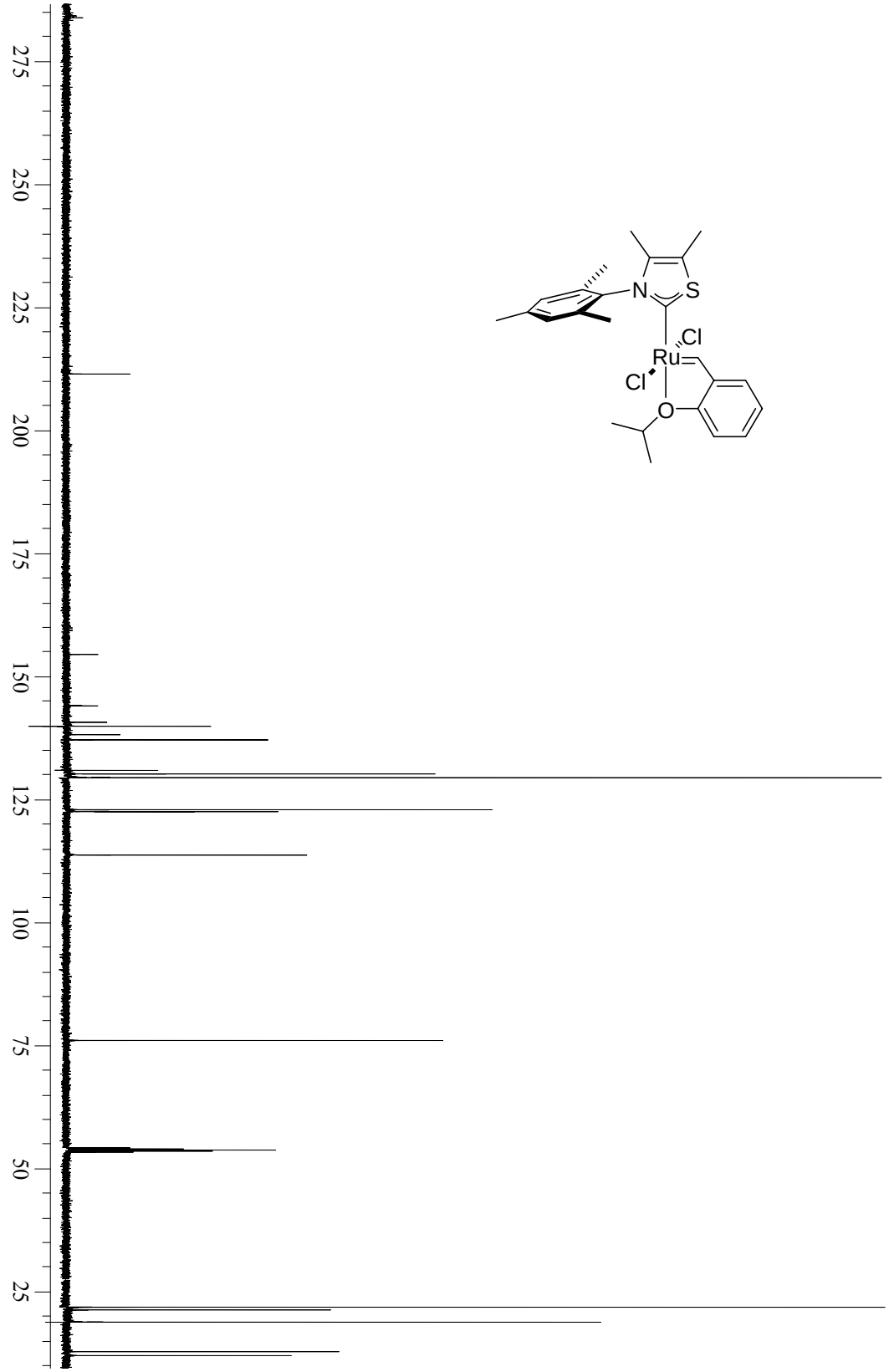
^{13}C NMR (CD_2Cl_2)



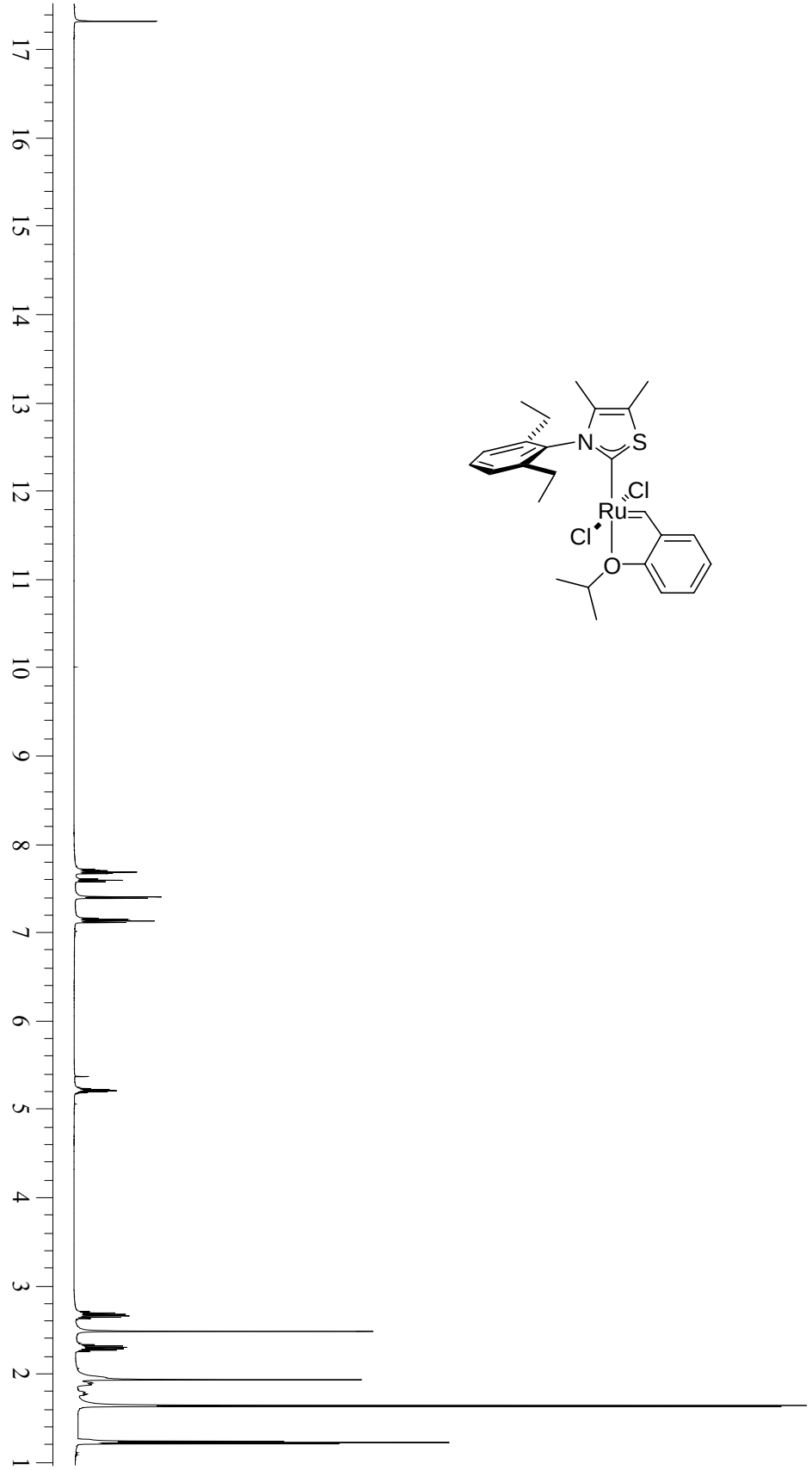
^{1}H NMR (CD_2Cl_2)



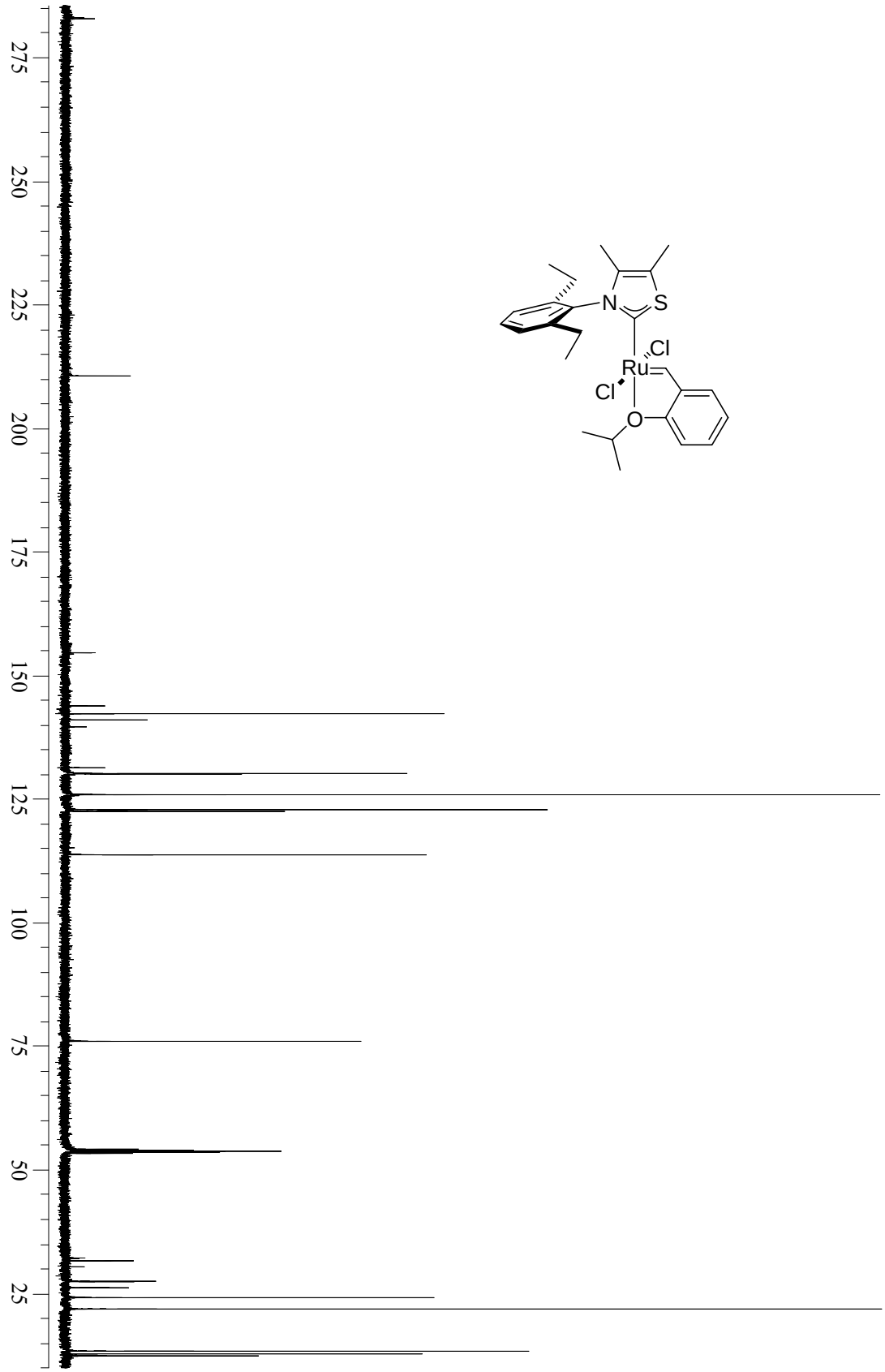
^{13}C NMR (CD_2Cl_2)



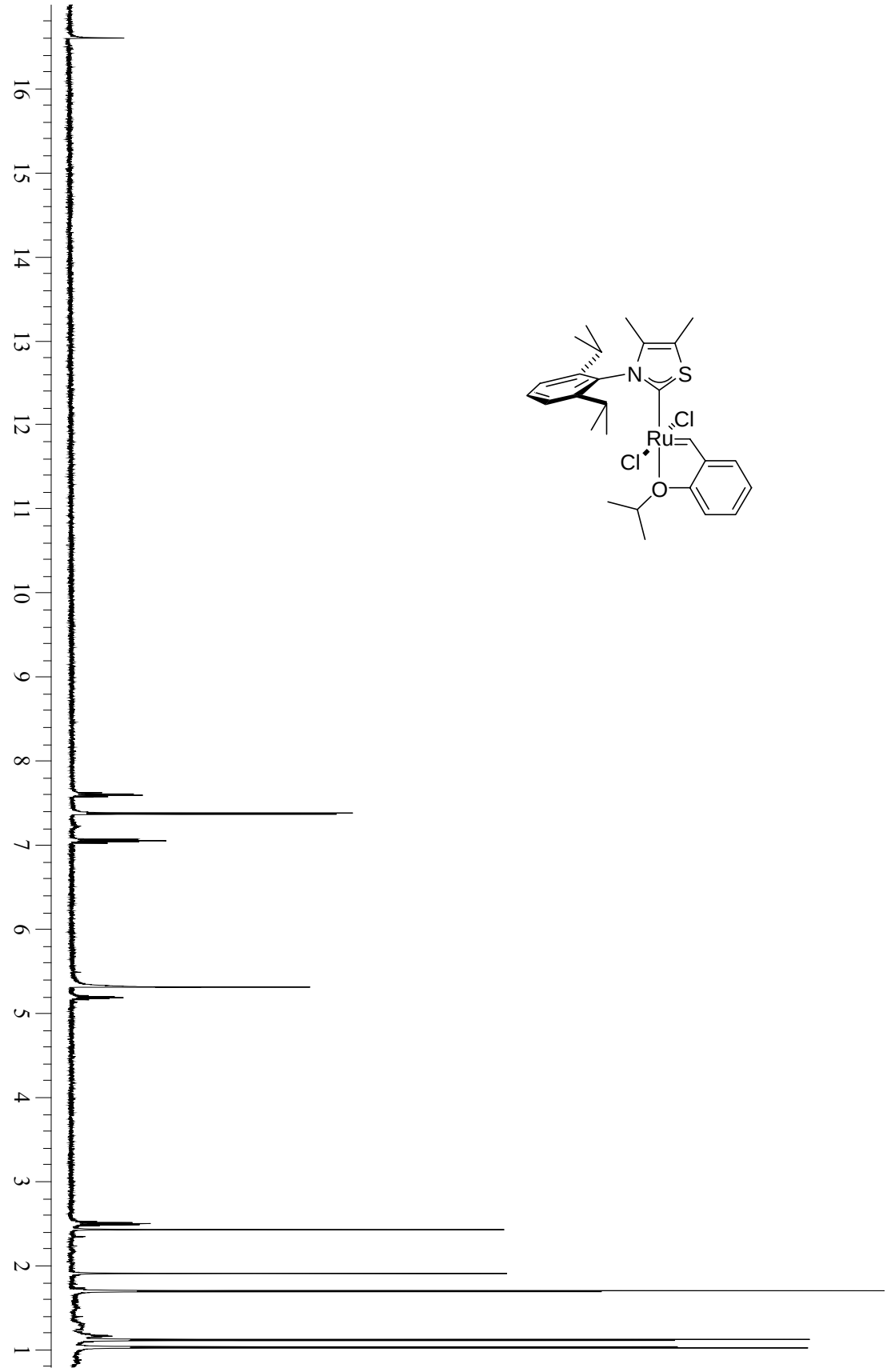
^{1}H NMR (CD_2Cl_2)



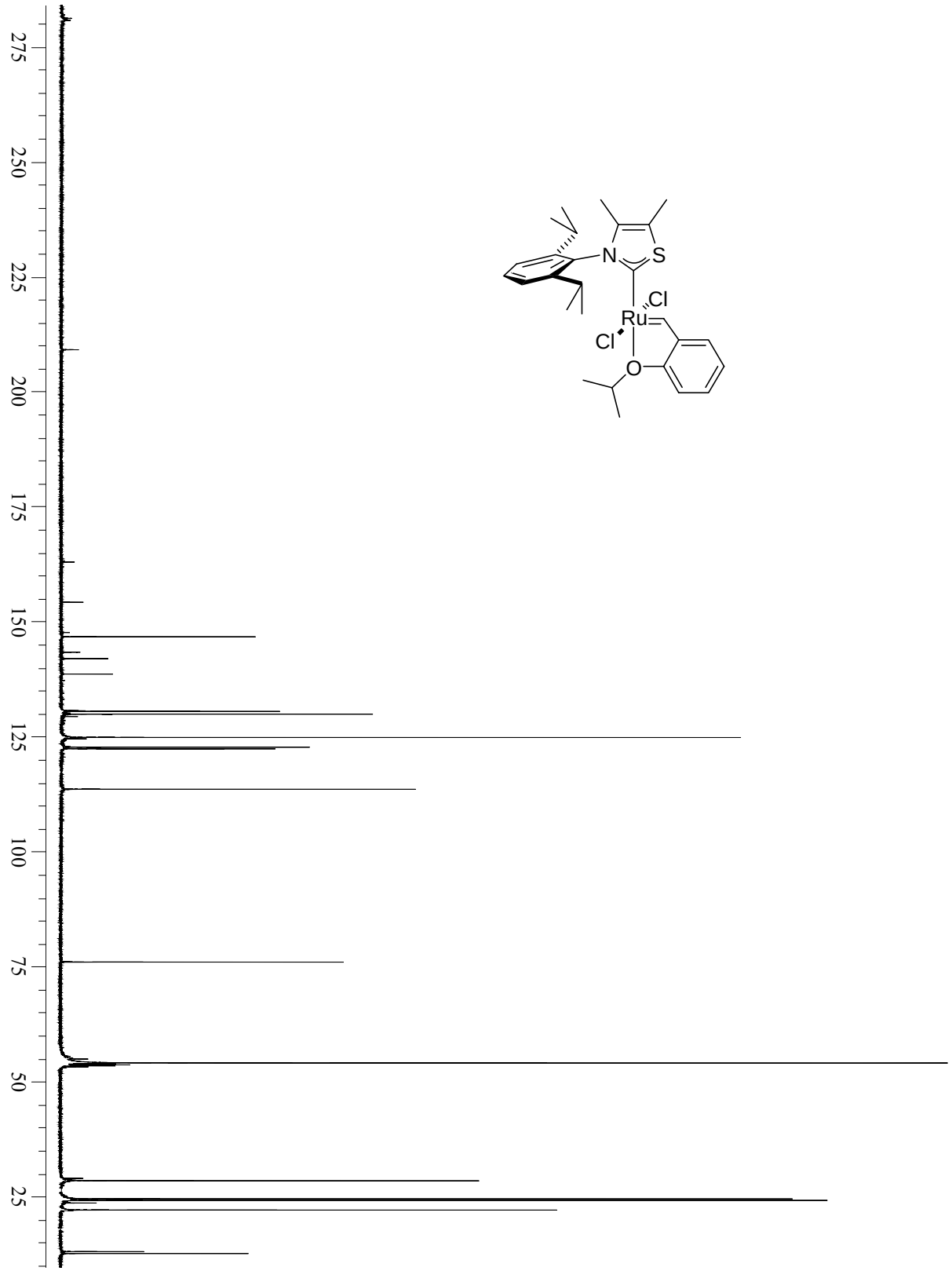
^{13}C NMR (CD_2Cl_2)



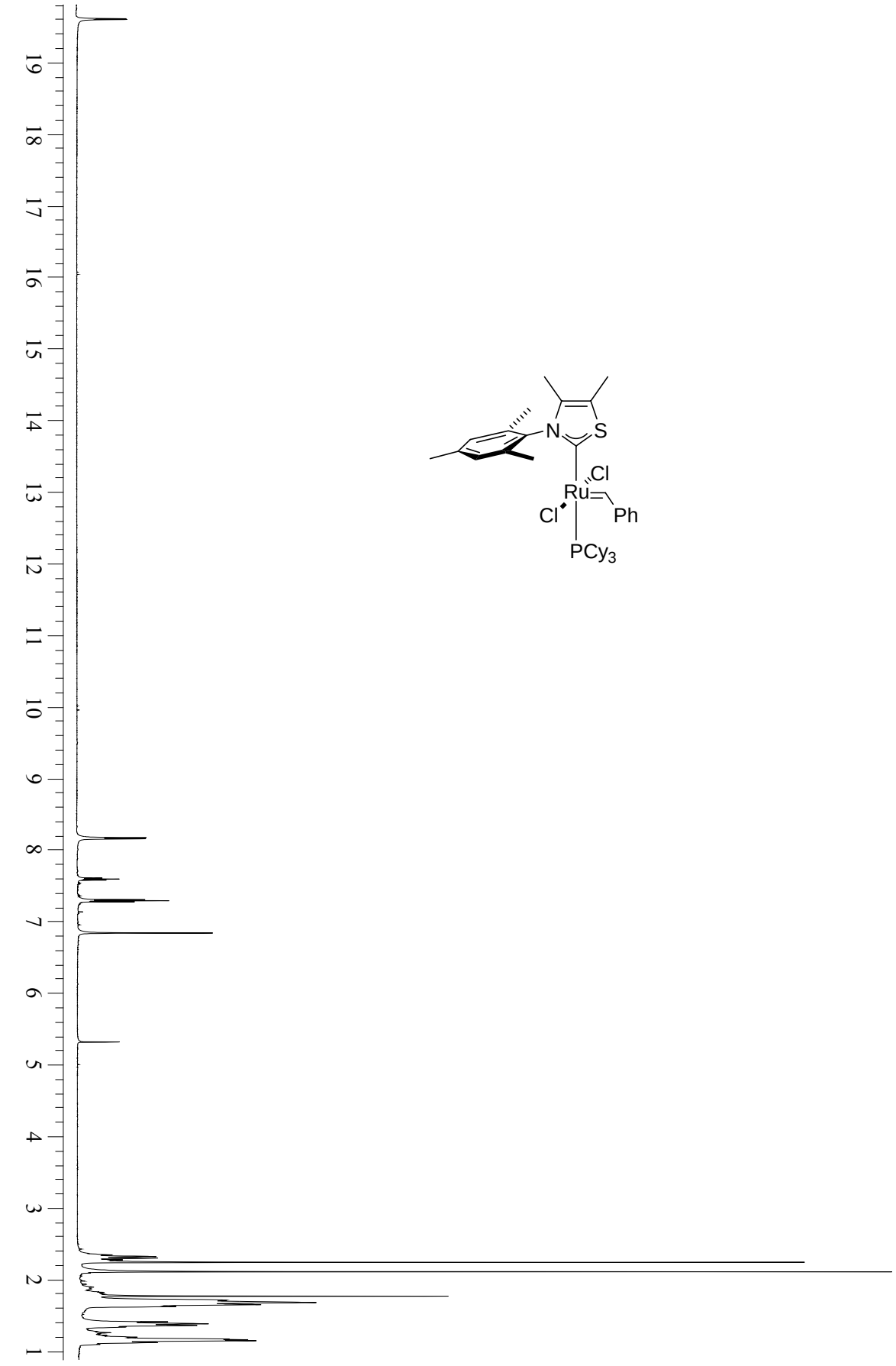
^{1}H NMR (CD_2Cl_2)



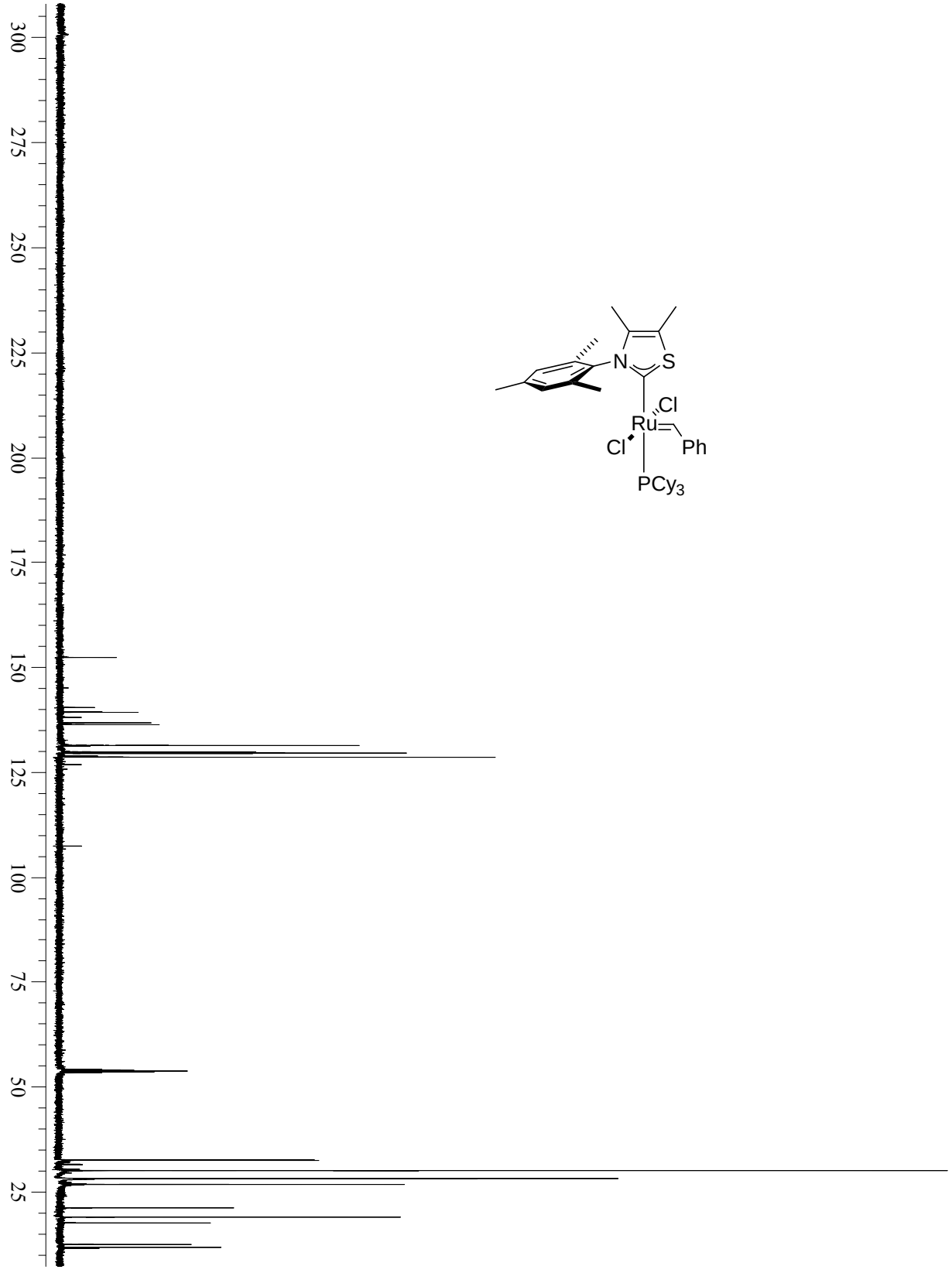
^{13}C NMR (CD_2Cl_2)



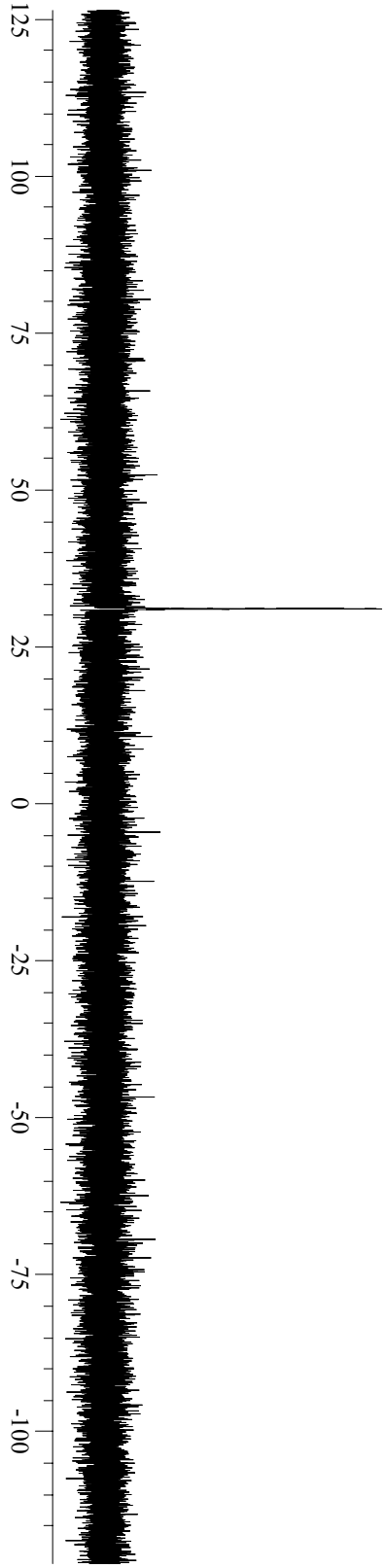
^{1}H NMR (CD_2Cl_2)

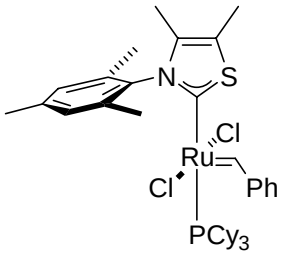


^{13}C NMR (CD_2Cl_2)

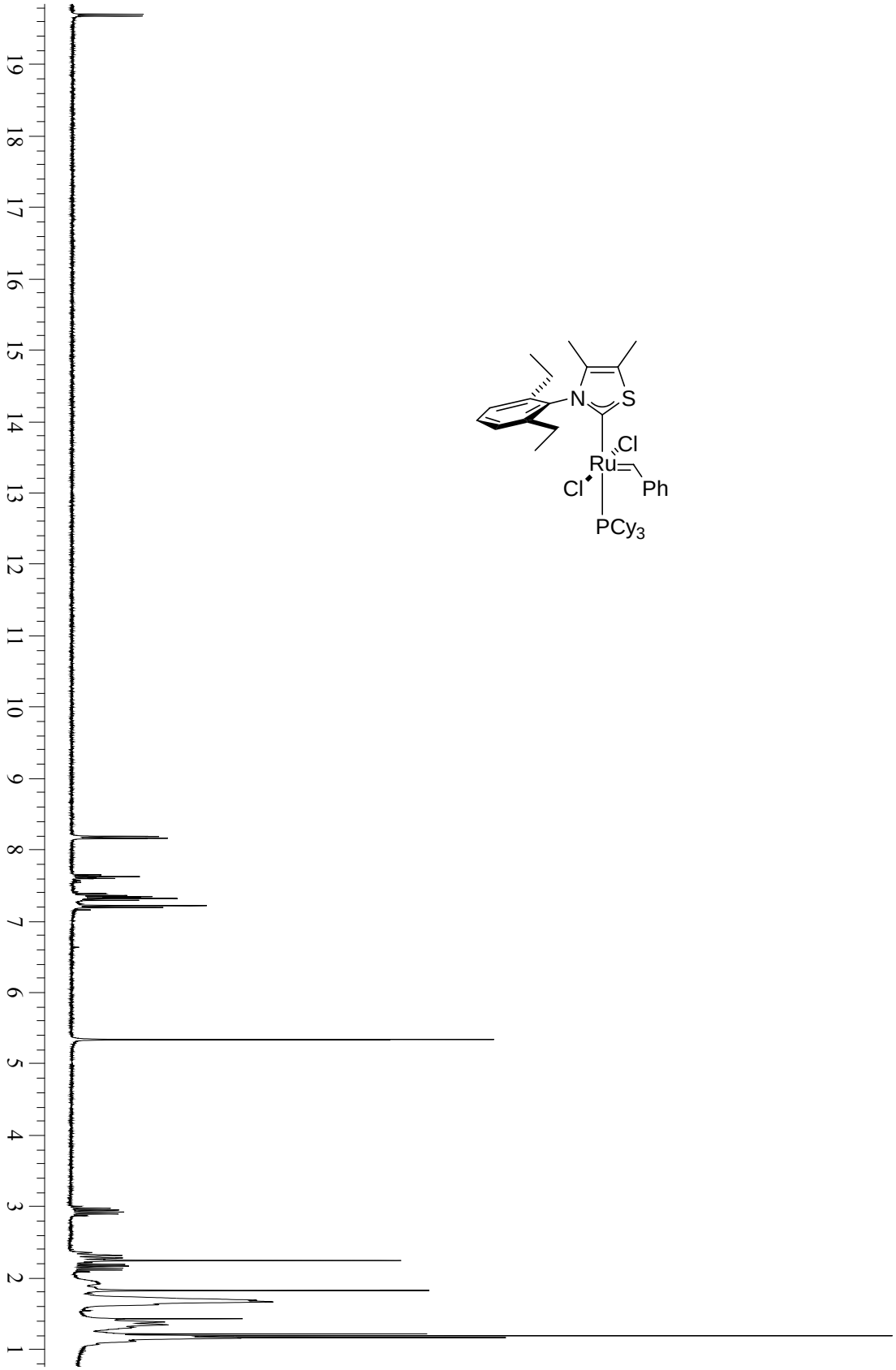


^{31}P NMR (CD_2Cl_2)

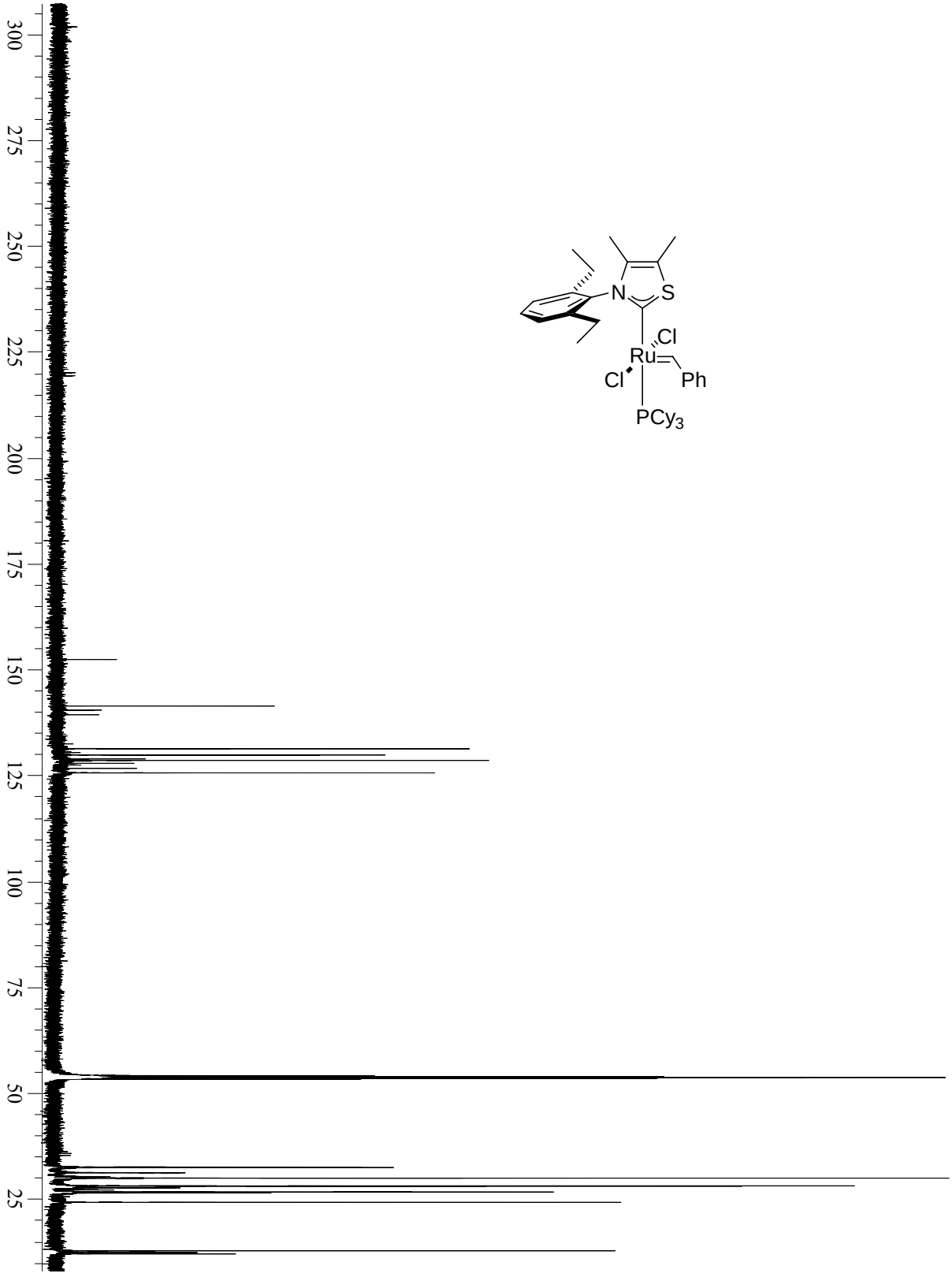




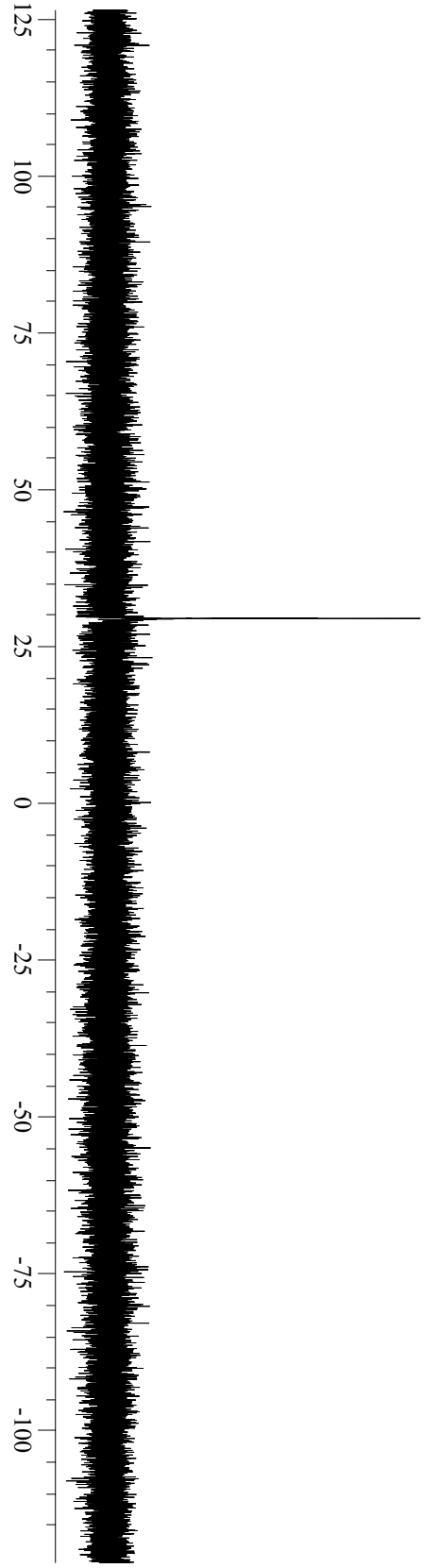
^{1}H NMR (CD_2Cl_2)

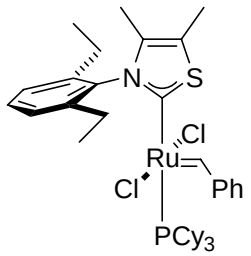


^{13}C NMR (CD_2Cl_2)

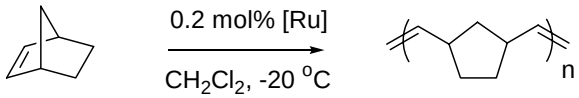


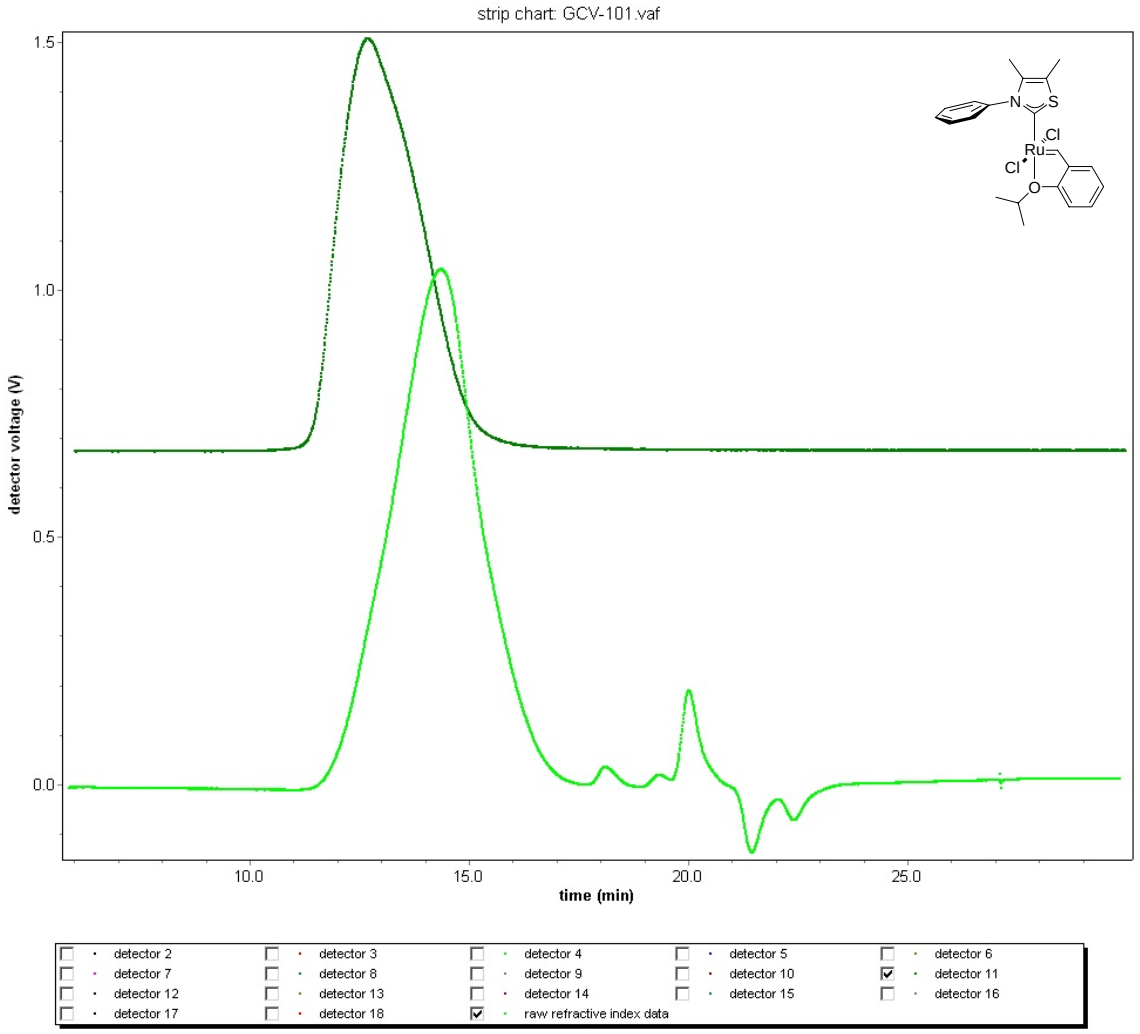
^{31}P NMR (CD_2Cl_2)

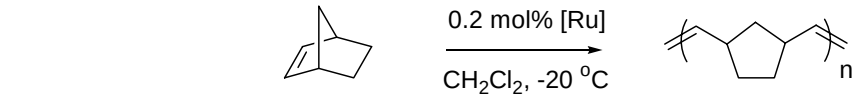


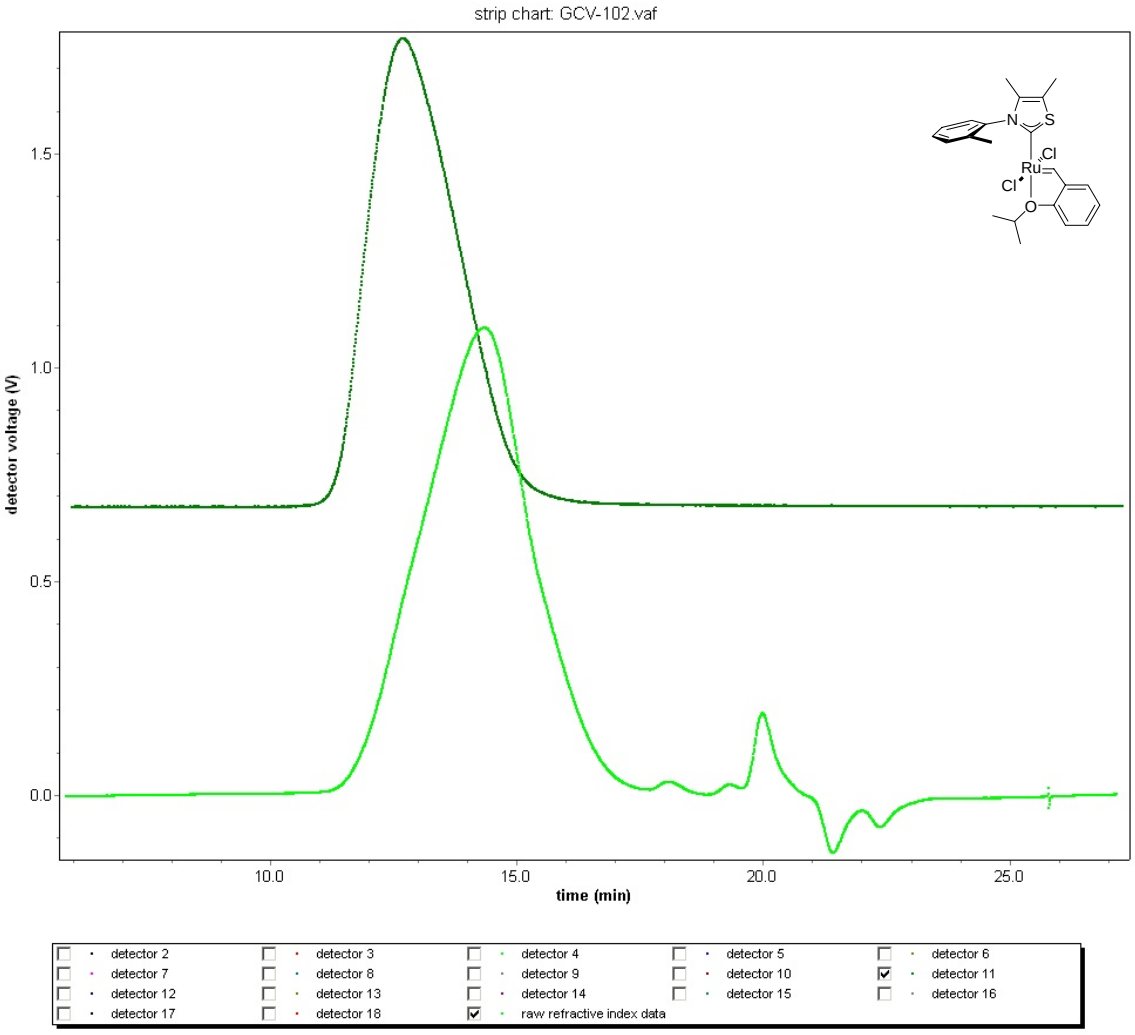


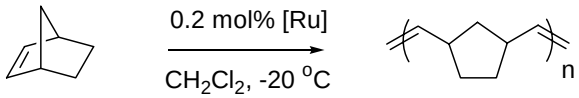
GPC Chromatograms (ROMP of norbornene)

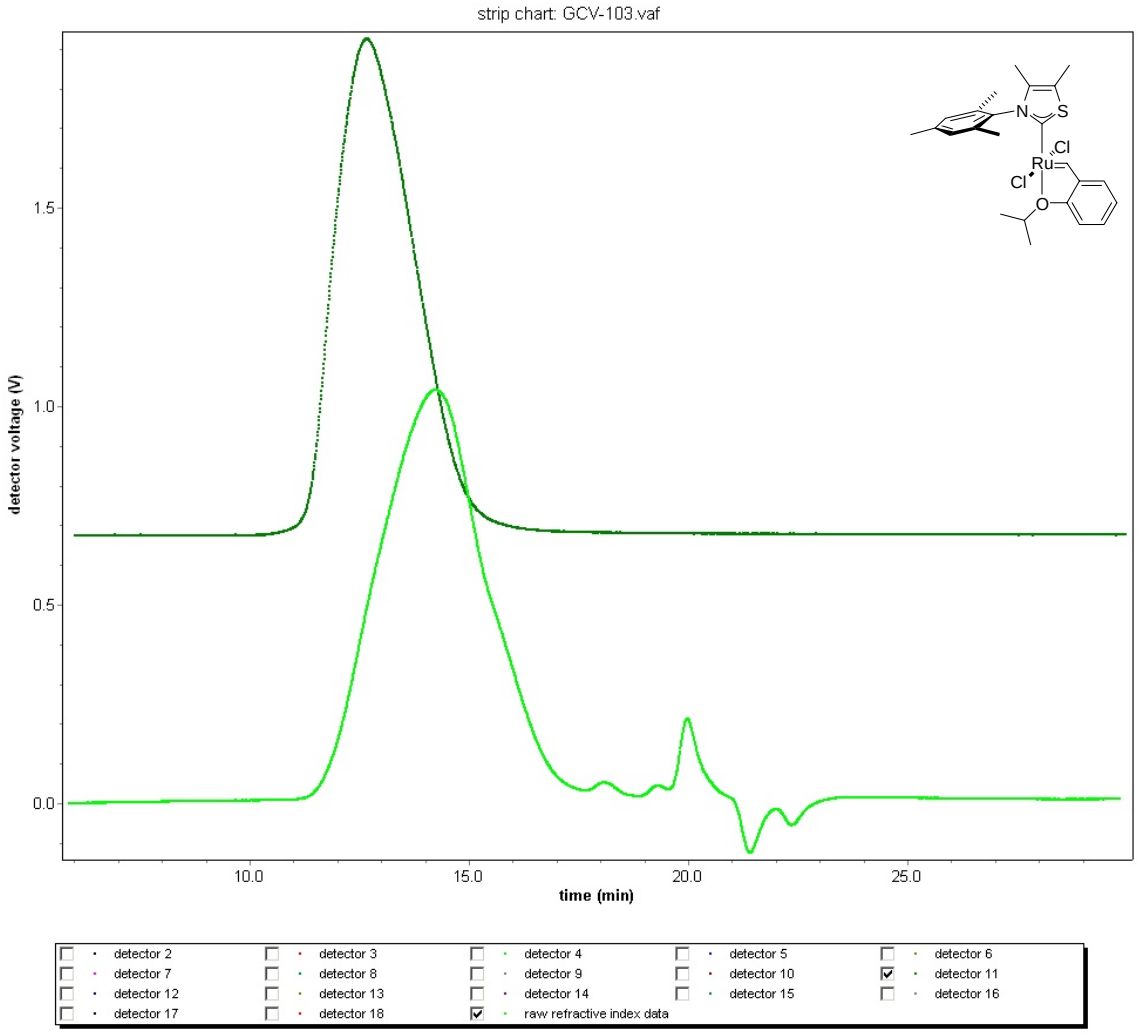


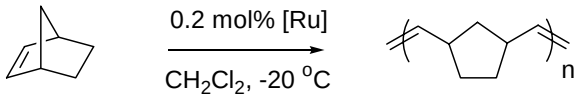


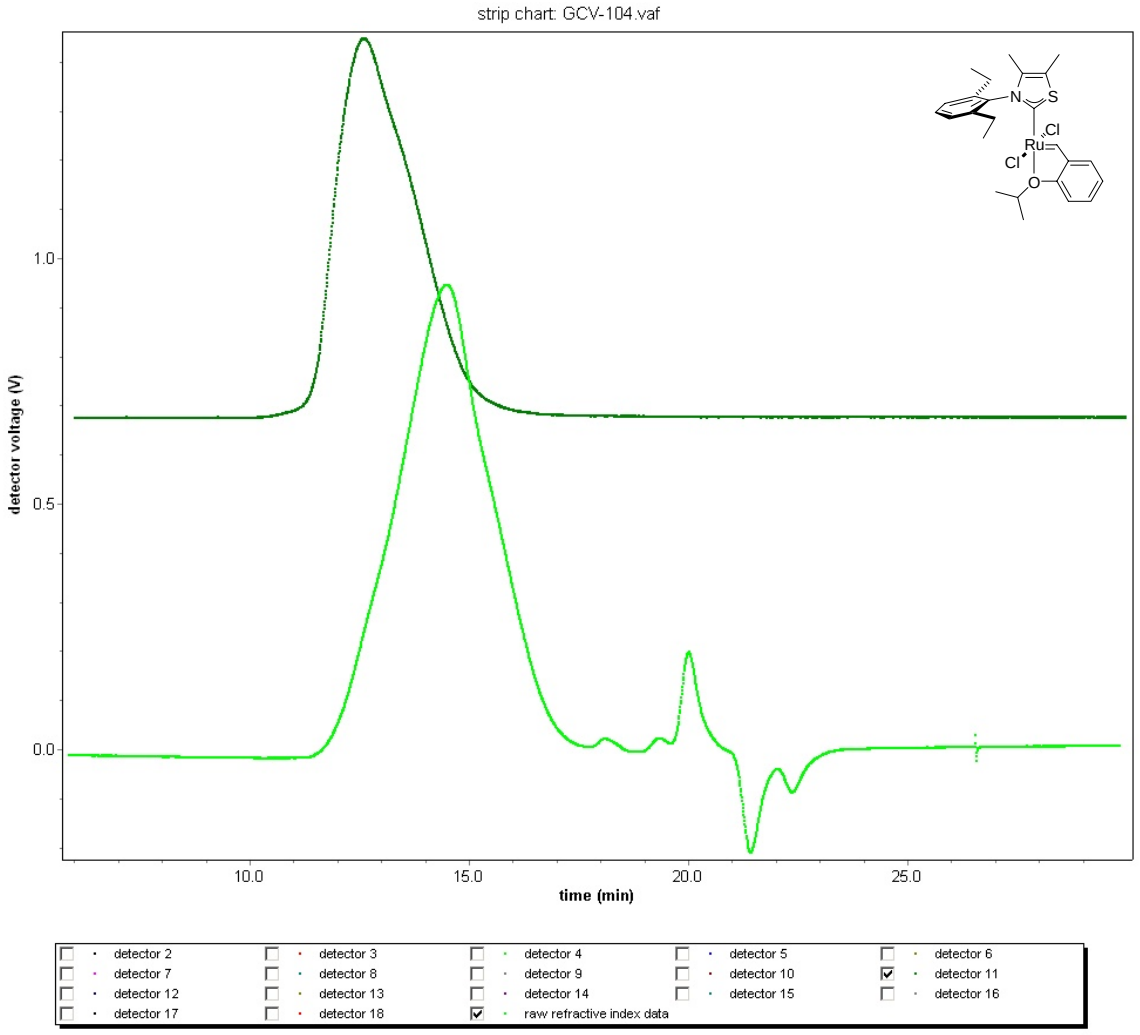

0.2 mol% [Ru]
CH2Cl2, -20 °C
n

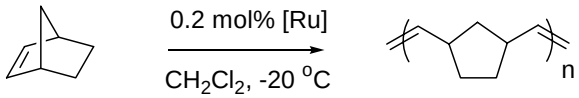

strip chart: GCV-102.vaf
detector voltage (V)
1.5
1.0
0.5
0.0
10.0
15.0
20.0
25.0
time (min)
N
S
Cl
Ru
Cl
O
detector 2
detector 3
detector 4
detector 5
detector 6
detector 7
detector 8
detector 9
detector 10
detector 11
detector 12
detector 13
detector 14
detector 15
detector 16
detector 17
detector 18
raw refractive index data

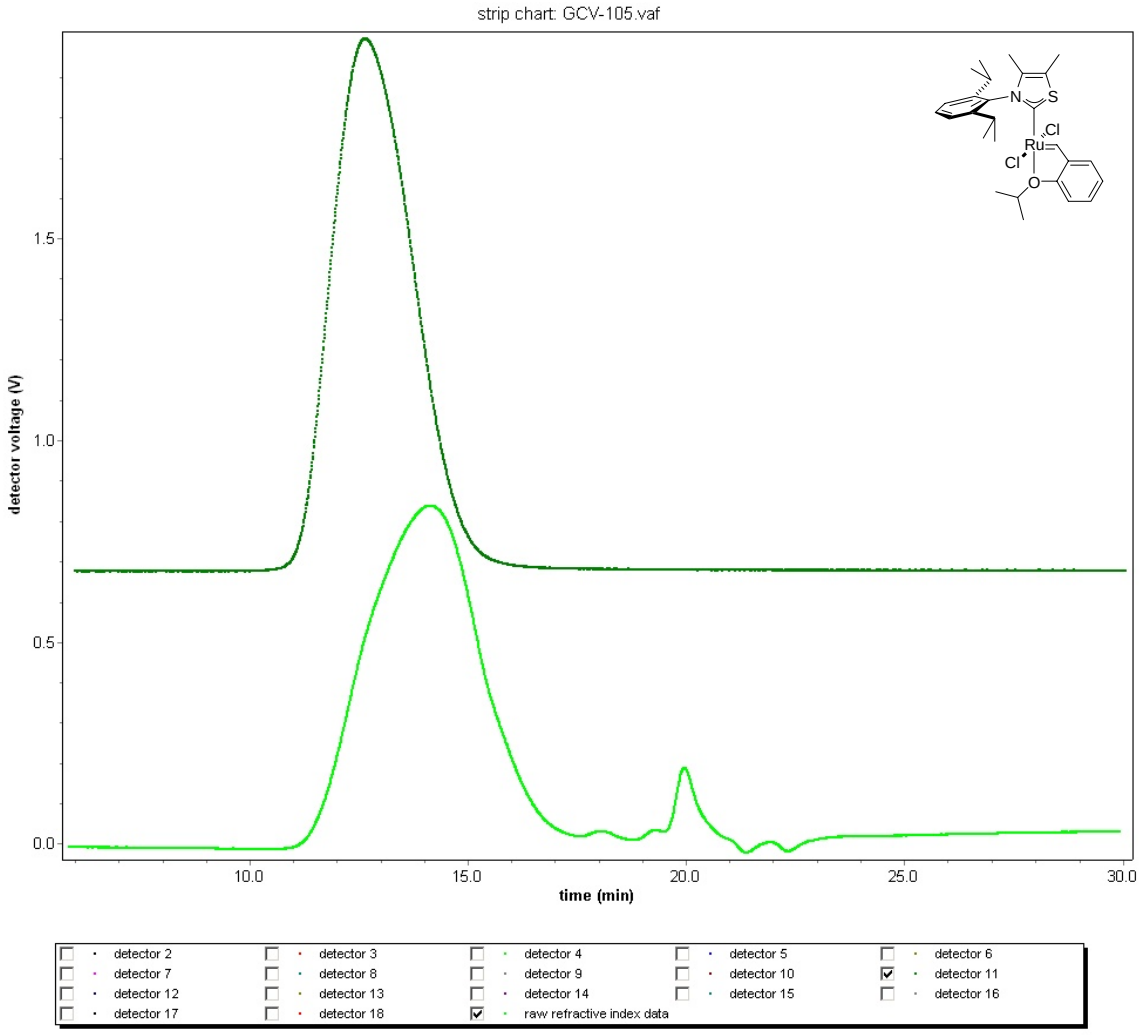

0.2 mol% [Ru]
CH_2Cl_2, -20 °C
n


strip chart: GCV-103.vaf
detector voltage (V)
1.5
1.0
0.5
0.0
10.0
15.0
20.0
25.0
time (min)
N
S
Cl
Ru
Cl
O
detector 2
detector 3
detector 4
detector 5
detector 6
detector 7
detector 8
detector 9
detector 10
detector 11
detector 12
detector 13
detector 14
detector 15
detector 16
detector 17
detector 18
raw refractive index data


0.2 mol% [Ru]
CH_2Cl_2, -20 °C
n

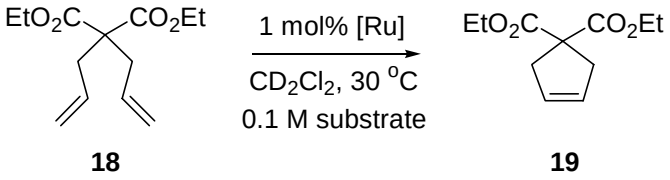

strip chart: GCV-104.vaf
detector voltage (V)
1.0
0.5
0.0
10.0
15.0
20.0
25.0
time (min)
N
S
Cl
Ru
Cl
O
detector 2
detector 3
detector 4
detector 5
detector 6
detector 7
detector 8
detector 9
detector 10
detector 11
detector 12
detector 13
detector 14
detector 15
detector 16
detector 17
detector 18
raw refractive index data


0.2 mol% [Ru]
CH_2Cl_2, -20 °C
n

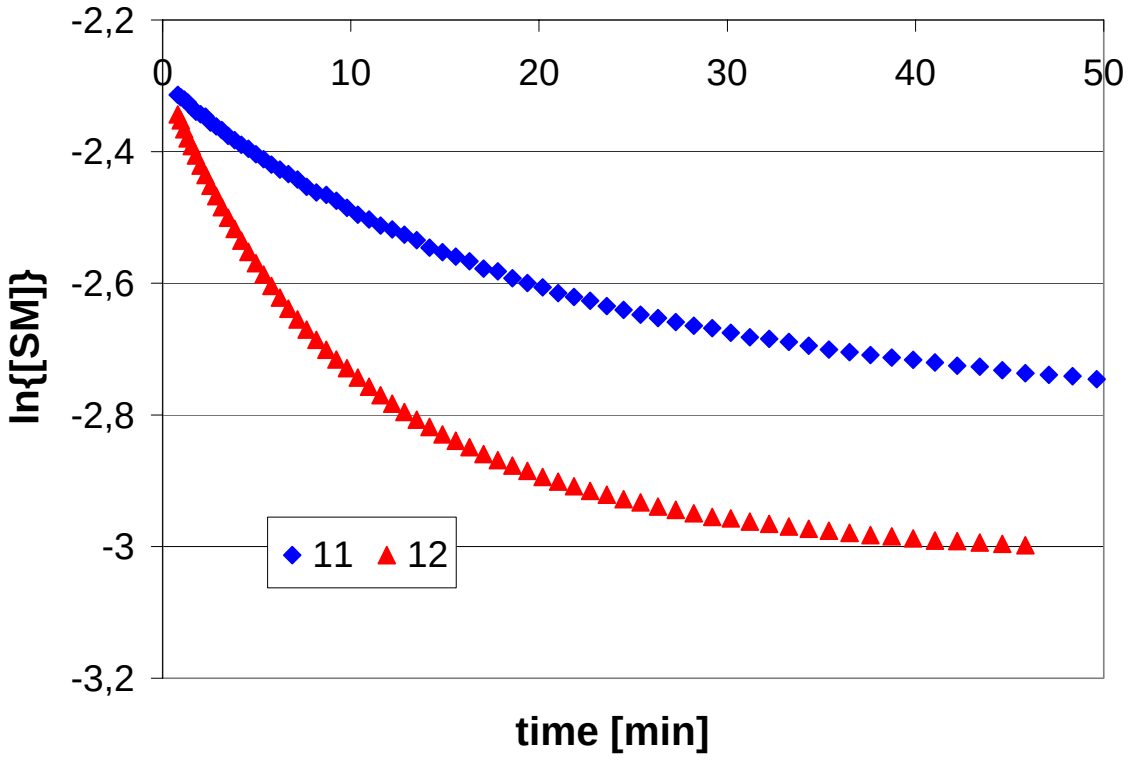

strip chart: GCV-105.vaf
detector voltage (V)
1.5
1.0
0.5
0.0
10.0
15.0
20.0
25.0
30.0
time (min)
N
S
Cl
Ru
Cl
O
detector 2
detector 3
detector 4
detector 5
detector 6
detector 7
detector 8
detector 9
detector 10
detector 11
detector 12
detector 13
detector 14
detector 15
detector 16
detector 17
detector 18
raw refractive index data

Catalytic Activity Evaluation Data

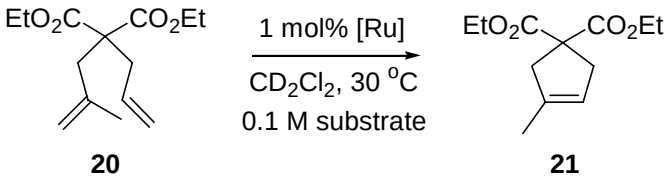
Decomposition of catalysts **11** and **12**:



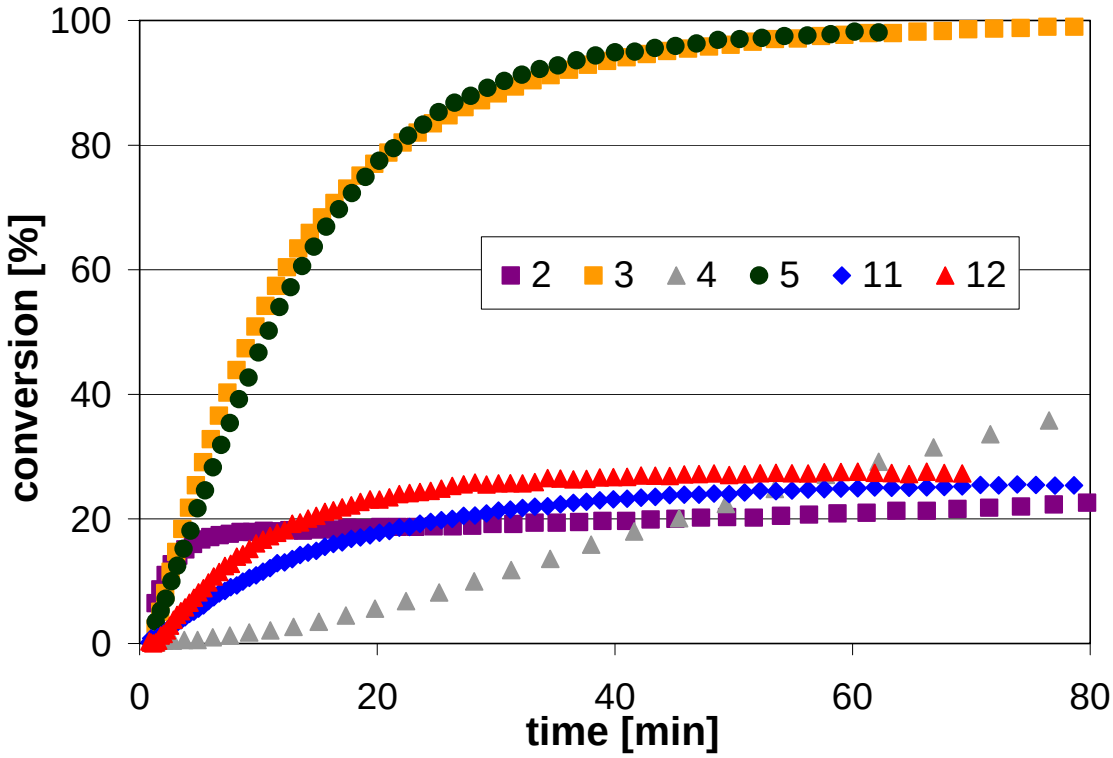
18 **19**



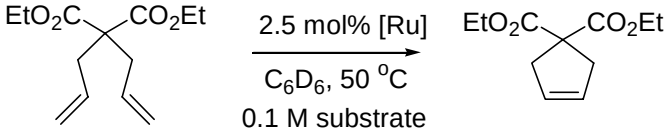
RCM of diethylallylmethallyl malonate:



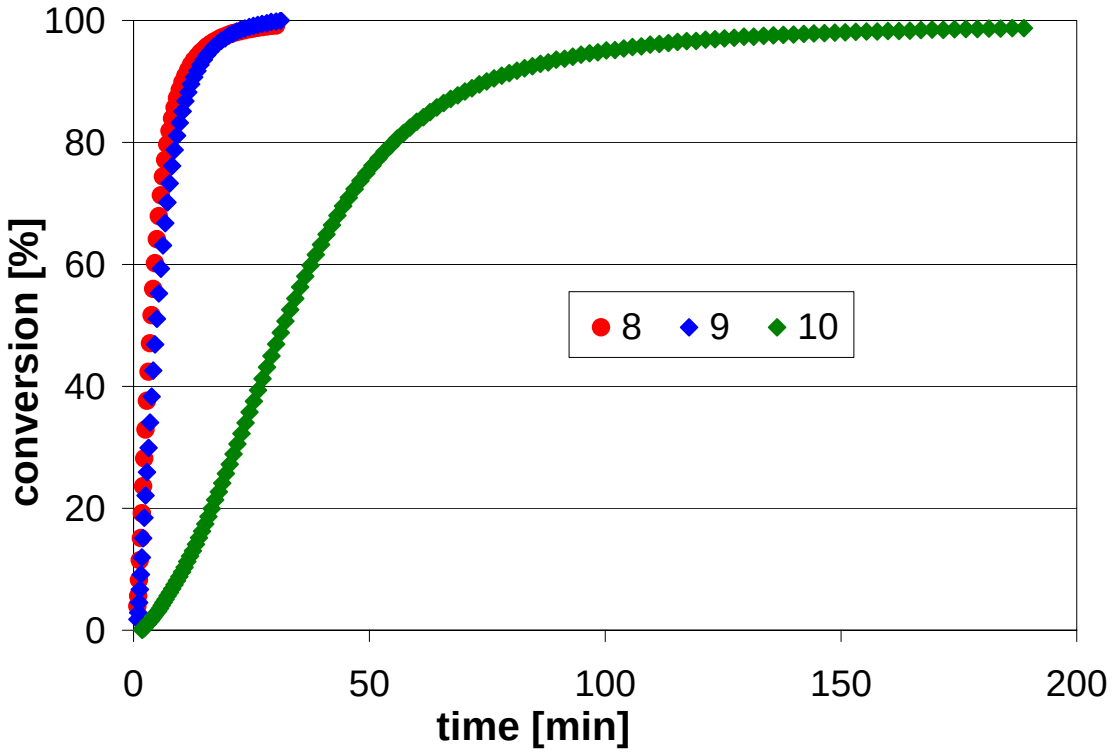
20 **21**



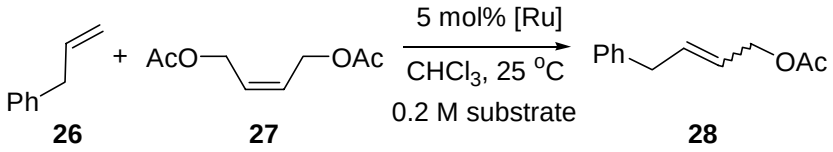
RCM of diethyldiallyl malonate:



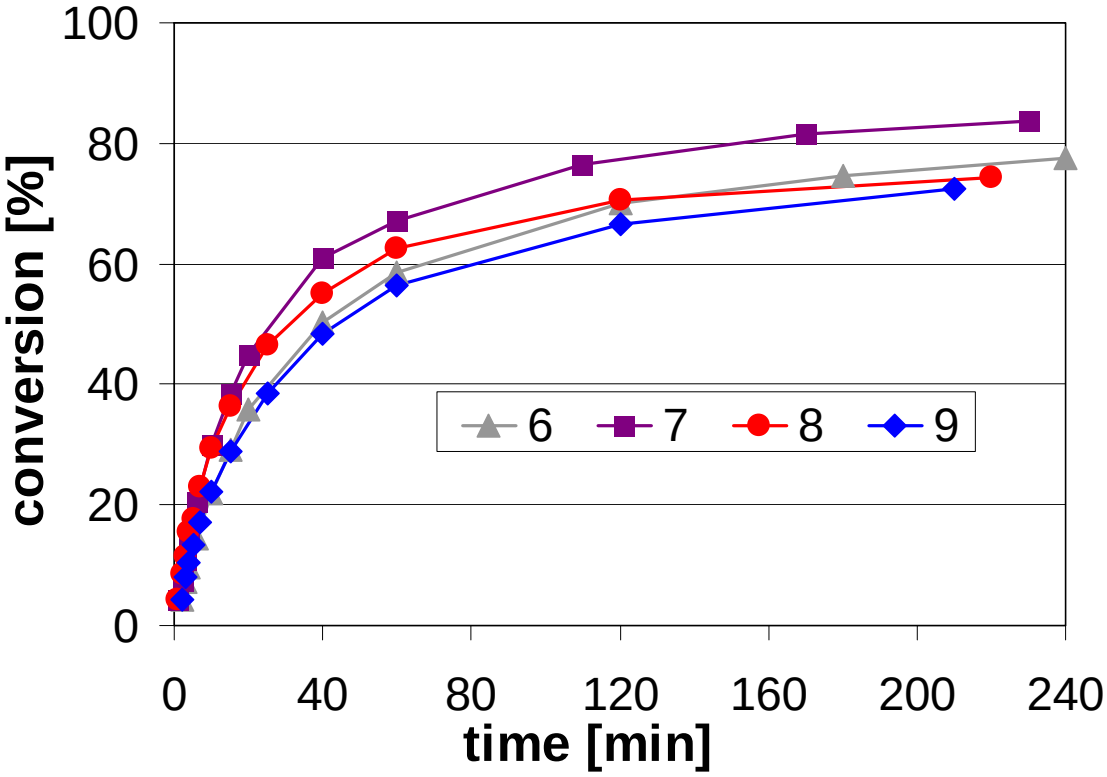
18 **19**



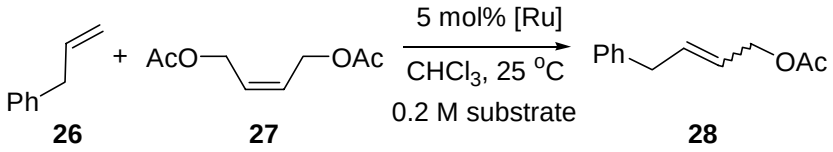
CM of allyl benzene with *cis*-1,4-diacetoxy-2-butene:



26 **27** **28**



CM of allyl benzene with *cis*-1,4-diacetoxy-2-butene:



26 **27** **28**